5th Conference on Elementary Processes in Atomic Systems

2nd National Conference on Electronic, Atomic, Molecular and Photonic Physics

CEPAS 2011 & CEAMPP 2011

CONTRIBUTED PAPERS
&
ABSTRACTS OF INVITED LECTURES

Editors

Aleksandar R. Milosavljević, Saša Dujko and Bratislav P. Marinković

Institute of Physics
Belgrade, Serbia

Belgrade, 2011

CONTRIBUTED PAPERS & ABSTRACTS OF INVITED LECTURES
of the
5th CONFERENCE ON ELEMENTARY PROCESSES IN ATOMIC SYSTEMS
and the satellite meeting
2nd NATIONAL CONFERENCE ON ELECTRONIC, ATOMIC, MOLECULAR AND PHOTONIC PHYSICS

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PREFACE

This book contains the Contributed papers and abstracts of the Invited lectures to be presented at the 5st Conference on Elementary Processes in Atomic Systems – CEPAS 2011 and 2nd National Conference on Electronic, Atomic, Molecular and Photonic Physics – CEAMPP 2011.

The Conference on Elementary Processes in Atomic Systems (CEPAS) is held triennially to promote the growth and exchange of scientific information in the field of photo-processes and laser collisions, electron (positron)/atom collisions, collisions with biomolecules, heavy particles (ion/atom) collisions, interactions with surfaces and processes with nano-sized complex systems. The first conference in the CEPAS series was organized in Uzhorod (Ukraine, 2000), the second one in Gdańsk (Poland, 2002), the third in Miskolc (Hungary, 2005), the forth in Cluj-Napoha (Romania, 2008) and the present fifth in Belgrade (Serbia, 2011). In all of these places, scientific research has been well established in particular fields that highlight the conference topics but the given opportunity to organize the CEPAS conference leads to further promotion of science and local research groups, thus receiving the full international recognition. The scientific program of the CEPAS 2011 consists of sessions of invited plenary (30 min) and topical (25 min) lectures. Contributed papers are presented as posters in afternoon sessions.

The National Conference on Electronic, Atomic, Molecular and Photonic Physics - CEAMPP is now a traditional national conference covering a wide range of scientific topics in atomic and molecular physics. The CEAMPP aims to bring together and support collaboration between different groups working basically in various fields of atomic and molecular physics, so to induce new ideas and interdisciplinary research. The focus of the CEAMPP is placed upon the young and distinguished researchers, who will be invited to give the most of the lectures at the conference. Still, the CEAMPP aims to preserve a high scientific level with the goal of presenting the frontier results both in Serbia and worldwide.

We are grateful for the support to Ministry of Education and Science of Republic of Serbia, Embassy of France in Belgrade, Embassy of Austria in Belgrade, Framework programme 7 project "Virtual Atomic and Molecular Data Centre" - VAMDC, Springer's journal "European Physical Journal D: Atomic, Molecular, Optical and Plasma Physics". We also acknowledge the support of Serbian Academy of Science and Arts and Institute of Physics, University of Belgrade. Finally, we are also grateful to Astra travel agency for technical organization of the conference.

The Editors would like to thank the members of the International Advisory Board of CEPAS 2011 and Scientific Committee of CEAMPP 2011 for their efforts in proposing the program of the conference, as well as plenary and topical invited lectures. Finally, we acknowledge the support of all members of the Organizing Committee who contributed to the preparing and running of the conference.

The participants have been asked to send their papers in a format already prepared for publication. After peer review of contributions, the basic corrections have

been made to meet general form of the book and to avoid, as much as possible, typing, spelling and grammatical errors. The Editors apologize for all mistakes that emerged from the preparation process and software problems in the process of printing.

Finally we would like to thank all the invited speakers and the participants for taking part in CEPAS 2011 and CEAMPP 2011 and to wish them to have a pleasant stay in Belgrade.

Belgrade, June, 2011 Editors

ACKNOWLEDGEMENT

5th CONFERENCE ON ELEMENTARY PROCESSES IN ATOMIC SYSTEMS
&
2nd NATIONAL CONFERENCE ON ELECTRONIC, ATOMIC, MOLECULAR AND PHOTONIC PHYSICS

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CONFERENCE TOPICS

CEPAS 2011

1. Photo-processes and laser collisions
2. Electron(positron)/atom collisions
3. Collisions with biomolecules
4. Heavy particles (ion/atom) collisions
5. Interactions with surfaces
6. Processes with nano-sized complex systems

CEAMPP 2011

1. Atomic and Molecular Structure and Properties
2. Collision Processes
3. Photon Interaction with Atoms and Molecules

CEPAS 2011

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CEAMPP/ CEPAS 2011 PROGRAM

Tuesday 21st June 2011		
2nd National Conference on Electronic, Atomic, Molecular and Photonic Physics - CEAMPP		
*(**PL** – Plenary lecture: 25+5 min; **PR** – Progress report: 15+5 min)*		
08:00-09:15	Registration (CEAMPP)	
09:15-09:30	Opening (CEAMPP), Chair: Saša Dujko	
	***Plenary Session**, Chair: Aleksandar Milosavljević*	
09:30-10:00	*Dynamics of dissociative electron attachment to small molecules*	**Juraj Fedor**, University of Fribourg, Switzerland
10:00-10:30	*Soft X-ray spectroscopy of molecules and biomolecules*	**Christoph Nicolas,** SOLEIL Synchrotron, Saint-Aubin, France
10:30-11:00	*Grazing incidence fast atom diffraction on different materials*	**Nenad Bundaleski,** CEFITEC, Caparica, Portugal
11:00-11:30	***Coffee break***	
	***Session 2**, Chair: Saša Dujko*	
11:30-11:50	*On the propagation of positive streamers in N_2:O_2 mixtures*	**Gideon Wormeester,** CWI, Amsterdam, The Netherlands
11:50-12:10	*Numerical modeling of buffer gas positron traps*	**Srđan Marjanović,** Institute of Physics, Belgrade, Serbia
12:10-12:30	*Absolute cross sections for electron scattering from metal vapours*	**Sanja Tošić,** Institute of Physics, Belgrade, Serbia
12:30-12:50	*Excitation of molecules by low-energy electrons*	**Miroslav Ristić,** Faculty of Physics, Belgrade, Serbia
13:00-15:00	***Lunch break***	
	***Session 3**, Chair: Nenad Simonović*	
15:00-15:20	*Ab initio calculation of low-lying vibronic levels in the ground $X^2\Pi_u$ electronic state of dicyanoacetylene cation*	**Radomir Ranković,** Faculty of Physical Chemistry, Belgrade, Serbia
15:20-15:40	*Theoretical study of the Jahn-Teller effect*	**Maja Gruden Pavlović,** Faculty of Chemistry, Belgrade, Serbia
15:40-16:00	*Coherent effects in laser driven rubidium vapor*	**Milan Radonjić,** Institute of Physics, Belgrade, Serbia
16:00-16:20	*Monte Carlo modeling of Townsend discharges in hydrogen*	**Vladimir Stojanović,** Institute of Physics, Belgrade, Serbia
16:20-16:40	***Coffee break***	

16:45-18:00	Poster session (CEAMPP)	
18:00-19:00	Registration (CEPAS)	
19:00	***Welcome party for CEAMPP and CEPAS participants***	
Wednsday 22nd June 2011		
5th Conference on Elementary Processes in Atomic Systems - CEPAS		
*(**PL** – Plenary lecture: 30+5 min; **TL** – Topical lecture: 20+5 min)*		
08:00-08:45	Registration (CEPAS)	
08:45-09:00	Opening (CEPAS), Chair: Bratislav P. Marinković	
	***Plenary Session**, Chair: Zoran Lj. Petrović*	
09:00-09:35	*Positronium negative ion experiments*	**Yasuyuki Nagashima**, Tokyo University of Science, Japan
09:35-10:10	*Imaging electron/ion coincidences for gas phase photoionization studies of chiral systems on the DESIRS beamline at SOLEIL*	**Laurent Nahon**, SOLEIL synchrotron, France
10:10-10:40	***Coffee break***	
	***Session 2**, Chair: Nigel Mason*	
10:40-11:05	*Cross sections for elastic electron scattering from iodine*	**Michael Brunger**, Flinders University, Australia
11:05-11:30	*Quantum interferences in atomic ionization by short laser pulses*	**Diego Arbó**, Astronomia y Fisica del Espacio, Buenos Aires , Argentina
11:30-11:55	*Electron driven processes in biomolecules*	**Janina Kopyra**, University of Podlasie, Poland
11:55-12:20	*Multi- photon ionization of biomolecular clusters*	**Sam Eden**, The Open University, UK
12:30-15:00	***Lunch break***	
	***Session 3**, Chair: Robert DuBois*	
15:00-15:25	*Coherent wavepacket shaping in high Rydberg states*	**Shuhei Yoshida**, Vienna University of Technology, Austria
15:25-15:50	*Positron scattering from krypton*	**James Sullivan**, Australian National University, Australia
15:50-16:15	*Absolute differential cross sections for electron scattering from building blocks of biopolymers*	**Aleksandar Milosavljević**, Institute of Physics Belgrade, Serbia
16:15-16:35	***Coffee break***	

	***Session 4**, Chair: Viorica Stancalie*	
16:35-17:00	*Differential cross sections of some noble atoms studied by fast electron impact and inelastic x-ray scattering*	**Lin-Fan Zhu**, Hefei National Laboratory for Physical Sciences at Microscale, China
17:00-17:25	*The effect of temperature on guiding of slow highly charged ions through mesoscopic glass capillaries*	**Réka Bereczky**, ATOMKI, Debrecen, Hungary
17:30-19:00	***Poster session (1)***	
Thursday 23rd June 2011		
	***Plenary Session**, Chair: Friedrich Aumayr*	
09:00-09:35	*Effect of projectile coherence on atomic fragmentation processes*	**Michael Schulz**, Missouri University of Science and Technology, USA
09:35-10:10	*Collisions with biomolecules: negative ion formation*	**Paulo Limão-Vieira**, Universidade Nova de Lisboa, Portugal
10:10-10:40	***Coffee break***	
	***Session 2**, Chair: Paulo Limão-Vieira*	
10:40-11:05	*Hard X-ray polarimetry in energetic ion-atom collisions*	**Günter Weber**, Helmholtz Institute Jena, Germany
11:05-11:30	*Photoionization study of trapped biopolymer ions in the gas phase*	**Alexandre Giuliani**, SOLEIL synchrotron, France
11:30-11:55	*Spatially resolved transport properties for electrons in gases: Definition, interpretation, and calculation*	**Saša Dujko**, Institute of Physics Belgrade, Serbia
11:55-12:20	*Excitation reactions studied by electron induced fluorescence method*	**Juraj Országh**, Comenius University Bratislava, Slovakia
12:30-15:00	***Lunch break***	
	***Session 3**, Chair: Károly Tőkési*	
15:00-15:25	*On deviations from theory of electron-atom elastic scattering cross sections*	**Raymond Moreh**, Ben-Gurion University of the Negev, Israel
15:25-15:50	*Photofragmentation of organic molecules of biological interest*	**Paola Bolognesi**, CNR-IMIP, Italy
15:50-16:15	*Electron-impact and thermal fragmentation of the amino acid molecules: mechanisms and structure of the molecules*	**Alexander Snegursky**, Institute of Electron Physics Uzhgorod,Ukraine
16:15-16:40	*Nanostructures formed on various surfaces due to the impact of individual slow highly charged ions*	**Robert Ritter**, Vienna University of Technology, Austria
16:40-17:00	***Coffee break***	

17:00-18:30	**CEPAS Advisory Board meeting**	
19:30	***Concert***	
Friday 24th June 2011		
	***Plenary Session**, Chair: Bratislav P. Marinković*	
09:00-09:35	*Inelastic transitions of atoms (and molecules) induced by van der Waals interaction with a surface*	**Jacques Baudon**, University Paris 13, France
09:35-10:10	*Ions Colliding with Cold Polycyclic Aromatic Hydrocarbon Clusters*	**Patrick Rousseau**, CIMAP Caen, France
10:10-10:40	***Coffee break***	
	***Session 2**, Chair: Jiří Horáček*	
10:40-11:05	*Laser Raman scattering from biomolecules in nanoparticles-embedded tissue*	**Simona Cintă Pinzaru**, Babes-Bolyai University, Romania
11:05-11:30	*Scattering from biomolecules in helium droplets*	**Stefan Denifl**, University of Innsbruck, Austria
11:30-11:55	*Channeling of charged particles through carbon nanotubes*	**Duško Borka**, Vinča Institute of Nuclear Sciences, Serbia
11:55-12:20	*Resonant inelastic collisions of electrons with diatomic molecules*	**Karel Houfek**, Institute for Theoretical Physics Prague, Czech Republic
12:30-15:00	***Lunch break***	
	***Closing session**, Chair: Andrey Solov'yov*	
15:00-15:35	*Classical theory of atomic collisions – the first hundred years*	**Petar Grujić**, Institute of Physics Belgrade, Serbia
15:35-16:00	*Thermo-mechanical impact on biomolecules induced by heavy ions*	**Alexander V. Yakubovich**, Frankfurt Institute for Adv. Studies, Germany
16:00-16:25	*Ion Interactions with Graphene*	**Zoran Mišković**, University of Waterloo, Canada
16:30-16:50	***Coffee break***	
16:50-18:20	***Poster session (2)***	
20:00	***Conference dinner***	
Saturday 25th June 2011		
10:00	***Excursion***	

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Abstracts of Poster Contributions

CEAMPP 2011

Abstracts of Invited Plenary Lectures

Abstracts of Invited Progress Reports

Abstracts of Poster Contributions

5th Conference on Elementary Processes in Atomic Systems

PLENARY LECTURES

Imaging electron/ion coincidences for gas phase photoionization studies of chiral systems on the DESIRS beamline at SOLEIL

L. Nahon

Synchrotron SOLEIL, l'Orme des Merisiers, St Aubin BP48, 91192 Gif-sur-Yvette Cedex, France

Installed on the Synchrotron SOLEIL French facility, DESIRS is a undulator-based high resolution variable polarization beamline covering the VUV range (5-40 eV) [1]. Its scientific case is focused on VUV photon-induced processes in the valence shell, mainly on gas phase samples, via the study of photoabsorption (primary photochemical event) and the subsequent energy relaxation processes (photoionization, fragmentation). We aim at probing the molecular and electronic structures, the reactivity and (polarization-dependant) photodynamics on model or actual systems encountered in the universe, atmosphere and in the biosphere.

After a general introduction to the beamline, including a short description of our new wave-front division VUV Fourier-Transform absorption spectrometer, able to reach unprecedented 10^6 resolving power [2], I will present our imaging electron/ion coincidence spectrometer, DELICIOUS2 [3] based upon Velocity Map Imaging and Time-Of-Flight mass spectroscopy. This set-up allows to address both physical chemistry-related issues (ionization potentials, electronic structure, fragment appearance energies…) by recording with ultimate sub-meV resolution Threshold Photoelectron Spectra (TPES) in coincidence with mass-selected ions (TPEPICO), as well as more physics-related issues linked to the (fast) electron continuum in the photoionization process by the recording Angle-Resolved Photoelectron Spectra on mass-selected compounds (AR-PEPICO).

This latter mode of operation was used for the study of Photoelectron Circular Dichroism (PECD) which is observed as a forward/backward asymmetry, with respect to the photon axis, of the photoelectron angular distributions resulting from the circularly polarized light (CPL)-induced photoionization of pure gas phase enantiomers. PECD is already present in the pure E1 approximation leading to a very high relative intensity up to the few tens of % range. Besides, core- and valence-shell studies have shown that PECD is a strongly dynamical effect showing a rich photon energy dependence and also that it depends on the ionized orbital [4]. In addition, PECD proves to be a very sensitive probe of molecular conformation [5] and of the chemical environment [6], much more so than the ionization cross-sections or the usual β parameter.

After an introduction to this spectacular chiroptical effect in the double context of photoionization dynamics and potential analytical tool, I will present some recent results including a major Franck-Condon breakdown observed by vibrationally-resolved PECD, and the first angular parameter study on chiral mass-selected clusters [7]. Future prospects regarding the case of amino-acids as produced by thermal desorption of bio-aerosols [8] will be presented.

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Positronium negative ion experiments

Y. Nagashima

Department of Physics, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan

More than fifty years ago, J. A. Wheeler [1] proposed the existence of several kinds of exotic systems composed of three particles with equal masses and bound through Coulomb interaction. The positronium negative ion (Ps^-) is the only system that has been observed so far [2]. Although many theoretical studies have been achieved to explore the nature of Ps^-, measurements of the decay rate have been the only experiments for many years [3, 4], limited by the extremely weak Ps^- intensity.

In 2006, a new method of generating Ps^- was developed [5]. Some of slow positrons injected onto a clean tungsten surface lose their energy in the bulk, diffuse back to the surface and then are emitted as Ps^-. Although the formation efficiency observed was less than 0.01%, a dramatic enhancement of the efficiency to 1.25% has been achieved by coating Cs atoms onto the tungsten surface [6]. Furthermore, coating with Na has been found to be as effective for the Ps^- production and the effect stays longer [7].

This technique has enabled us to do new experiments. We have estimated the Ps^- binding energy experimentally by observing Ps^- emission from several kinds of metals coated with alkali metals [8]. We have also succeeded in the first observation of the photodetachment of the Ps^- [9], the cross sections of which have been calculated. The obtained lower limit of the photodetachment cross section for the wave length of 1064nm is consistent with the calculations. The Ps^- photodetachment technique can be used to produce an energy tunable Ps beam for future applications.

This presentation will give a review of the experimental studies performed so far and future plans of Ps^- experiments.

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Collisions with biomolecules: negative ion formation

P. Limão–Vieira

Laboratório de Colisões Atómicas e Moleculares, CEFITEC, Departamento de Física
FCT, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal
plimaovieira@fct.unl.pt

This is The dynamics of electron transfer processes in atom-molecule collisions are quite different from electron-molecule collisions. Only free electrons with an appropriate energy (resonance) can attach to the molecule for a time interval longer than around 10^{-16} s. This corresponds to the electron populating a discrete state of the molecule, with the incident energy matching the corresponding negative value of the Molecular Orbital (MO). In neutral atom-molecule collisions and subsequent ion pair formation, the electron is transferred when the wave function of the neutral atom plus molecule coincided with that of the atomic cation plus molecular anion. This only occurs at specific points of the reaction coordinate, known as the crossing radius (R_c). The required energy in these processes is given by the *endoergicity* for the electron transfer process: ΔE = IE(K)–EA(Molecule), with IE(K) the ionisation energy of the atom (potassium in this case) and EA(Molecule) is the electron affinity of the molecule. As such, electron will be transferred to a given MO of the molecule with the corresponding energy being provided by the collision.

Previous studies on DNA/RNA nucleobases [1], [2] support the efficient auto-detachment of electrons from the orbitals that are responsible for the breaking of ring bonds. We propose that the third body in the present experiments (the potassium cation) may act as a stabilizing agent, suppressing auto-detachment and hence allowing more efficient electron transfer to the ring-breaking σ^* orbitals [3], [4], [5]. A similar reduction in auto-detachment has previously been demonstrated for low energy Rydberg atom-molecule collisions [6], [7].

The aim of this presentation is to show and analyse anion production from thymine, uracil and some halouracils due to electron transfer from potassium atoms in the context of the available free electron attachment data, quantum chemical calculations, and collision theory. As the outermost electron is weakly bound in potassium, the results can provide insights relevant to electron transfer processes from electronically excited secondary neutrals in irradiated biological material. From a more fundamental point of view, the present work probes charge transfer to the most complex polyatomic molecules yet studied in fast collisions with atoms. Hence it can provide general dynamical information to enhance our understanding of these types of collisions, notably regarding intramolecular electron transfer processes coupled with the non-adiabatic atom-molecule electron transition.

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Effect of projectile coherence on atomic fragmentation processes

M. Schulz[a], K. Egodapitiya[a], S. Sharma[a], A.C. Laforge[a,b], R. Moshammer[b], A. Hasan[c], D.H. Madison[a]

[a]*Missouri S&T Roll, USA*
[b]*MPI-K, Germany*
[c]*UAE University, UAE*

Several years ago a surprising symmetry breaking, strictly demanded by first-order theories, was reported in measured fully differential cross sections (FDCS) for single ionization by ion impact even for very small perturbation parameters η (projectile charge to speed ratio) [1]. Until today, the data could not even qualitatively be reproduced by any fully quantum-mechanical calculation. In contrast, treating the projectile – target nucleus interaction classically resulted in good agreement with the data [2]. This raises the question whether the fully quantum-mechanical calculations share a fundamental problem which has been overlooked so far. One feature which all of these calculations have in common is that they assume a completely de-localized projectile wave, i.e. a coherent projectile beam. This is a very unrealistic assumption for fast ion impact since there the projectile wave packet always has a width which is negligible compared to the size of the target atom. Here, we report experimental data which demonstrate that cross sections for atomic fragmentation processes can sensitively depend on the projectile coherence.

We measured the fully momentum-analyzed scattered projectiles in coincidence with the recoiling target ions for ionization in 75 keV p + H_2 collisions. From the data we extracted double differential cross sections (DDCS) for a fixed projectile energy loss of ε = 30 eV as a function of scattering angle θ. The width of the projectile wave packet (i.e. the transverse coherence length Δr) is proportional to $L\lambda/a$, where L is the distance between the collimating slit and the target region, a is the slit width, and λ the DeBroglie wave length of the projectile. The experiment was performed for L_1=50 cm and L_2=6.5 cm, which for a=0.15 mm corresponds to $\Delta r \approx$ 2 a.u. and 0.3 a.u., respectively.

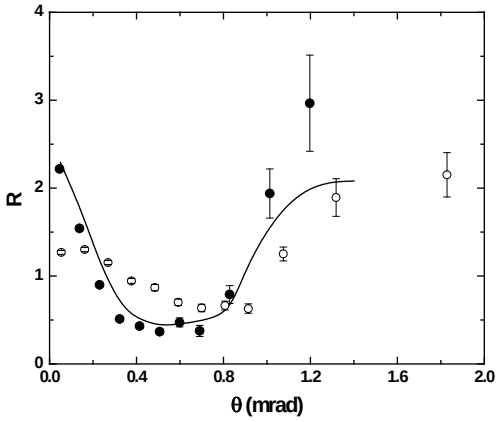

Fig.1. Cross section ratio for large to small slit distance for ionization (closed symbols) and capture (open symbols). Curve: theory for ionization

In the DDCS for L_1 we observe a pronounced interference structure, which is completely absent for L_2. The interference is due to indistinguishable diffraction of the projectile wave from the two atomic centers in the molecule [3]. However, it can only occur if the projectile wave packet is wide

enough to illuminate both atomic centers simultaneously, i.e. if $\Delta r > D$ (inter-nuclear separation). This explains why the interference is absent for L_2 since there $\Delta r < D$.

The closed symbols in Fig. 1 show the ratio R between the DDCS for L_1 and L_2, which, under the assumption that at L_2 the projectile beam is incoherent, to a good approximation represents the interference term. The solid curve shows a calculation of the DDCS assuming a coherent beam normalized to twice the DDCS for atomic hydrogen. Except for large θ this calculation qualitatively reproduces the experimental data.

The finding that the interference structure disappears for an incoherent projectile beam we recently confirmed by equivalent data for capture in 75 keV p + H_2 collisions (open symbols in Fig. 1). We thus have to conclude that it is crucially important to properly account for the projectile coherence length in theoretical calculations.

For atomic targets the unrealistic assumption of a coherent beam probably results in artificial path interference between two impact parameters leading to the same scattering angle. This could quite possibly explain the theoretical difficulties in reproducing measured FDCS for single ionization by fast ion impact. Indications for such path interference we observed for capture in 25 keV p + H_2 collisions for a coherent projectile beam, which again is not present for an incoherent beam.

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Inelastic transitions of atoms (and molecules) induced by van der Waals interaction with a surface

J. Baudon[a], M. Hamamda[a], M. Boustimi[b], V. Bocvarski [c],T. Taillandier-Loize[a], G. Dutier[a], F. Perales[a] and M. Ducloy[a]

[a]Laboratoire de Physique des Lasers, CNRS-UMR 7538, Université Paris 13, Villetaneuse, France ;[b]Oumm Al-Qura Universty, Mekkah, Saudi Arabia ; [c] Institute of Physics, Belgrade, Serbia

Making pass metastable atoms or molecules in the vicinity of a solid surface, as the slit edges of a micrometric or nanometric transmission grating, is a powerful experimental tool to enhance and better observe interactions with the surface, especially *via* inelastic transitions and their dynamical effects. At distances Z of a few ten nm, large enough to avoid any quenching by the solid, and small enough to make negligible retardation effects, the interaction is of the van der Waals (vdW) type, in Z^{-3}. Either because of non-zero internal momentum (for atoms) or internal rovibrational degrees of freedom (for molecules), the vdW interaction is not purely scalar but contains, for atoms in a P-state, an additional quadrupolar (anisotropic) term and, for molecules, a part depending on both the orientation of the molecular axis and the vibration coordinate. In general this anisotropic part of the interaction is responsible for a variety of inelastic processes. As the interaction involves the only coordinate normal to the surface, the momentum component parallel to the surface is conserved whereas the kinetic energy is changed. The resulting deflection allows the identification of the process. For metastable atoms (except He*), fine structure exo-energetic transitions as $^3P_0 \rightarrow {}^3P_2$ and the reverse process have been observed [1]. Within a magnetic field not normal to the surface, exothermal transitions among Zeeman sublevels called "van der Waals - Zeeman transitions" [2] occur (see figure 1). For metastable N_2* molecules, vibrational excitation and de-excitation ($\Delta v = \pm 1, 2$) have been also observed [3].

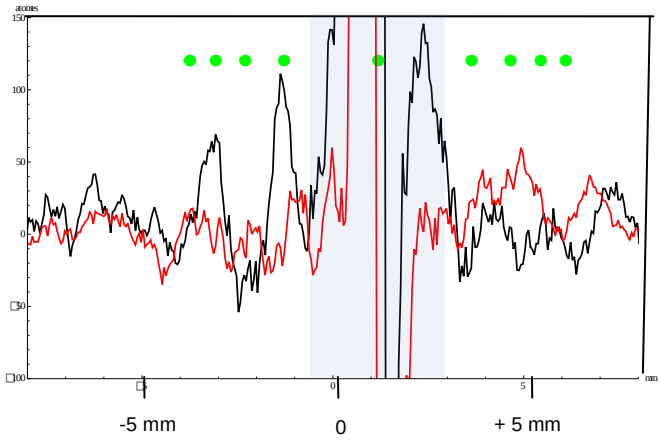

Fig.1. Example of vdW-Z transitions of Kr*($^3P_2$) atoms traversing a gold nano-grating. The shaded area is a non-observable domain. The red line is the base line of the signal. Full circles : predicted positions of the inelastic peaks on a position-sensitive detector located at 430 mm from the grating.

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Ions colliding with cold polycyclic aromatic hydrocarbon clusters

P. Rousseau[a], A. I. S. Holm[b], A. Ławicki[a], H. Zettergren[b], M. Capron[a], H. A. B. Johansson[b], E. Lattouf[a], S. Maclot[a], R. Maisonny[a], F. Seitz[b], A. Domaracka[a], A. Méry[a], J.-C. Poully[a], J. Rangama[a], S. Rosén[b], H. T. Schmidt[b], L. Adoui[a], B. Manil[c], H. Cederquist[b], B. A. Huber[a]

[a]*CIMAP, CEA/CNRS/ENSICAEN/Université de Caen Basse-Normandie, Boulevard Henri Becquerel, F-14070 Caen cedex 5, France*
[b]*Department of Physics, Stockholm University, SE-106 91 Stockholm, Sweden*
[c]*LPL, CNRS/Université Paris 13, Institut Galilée, 99 Avenue J. B. Clément, F-93430 Villetaneuse, France*

Polycyclic Aromatic Hydrocarbon (PAH) molecules are formed by fused carbonic aromatic rings, mostly benzenic ring. They are large π-electron systems with a large delocalization of the electrons over the molecule. PAHs typically exhibit a planar honeycomb structure; they can be considered as small hydrogen-saturated fragments of graphene.

PAH clusters are stacked structures of molecules bound by van der Waals interaction. As by-product of combustion processes, they represent an intermediate step in the formation of soot. In addition to the atmospheric interest, PAH molecules and clusters are supposed to be widely present in the interstellar medium. They are considered the sources of the aromatic bands in the mid-infrared emission spectra. Moreover, PAH clusters could constitute the very small grains observed in the interstellar medium. Therefore, PAH molecules and clusters could represent up to 20% of the interstellar carbon and thus could play a prime role in the physics and chemistry of the interstellar medium [1]. Despite this potential importance, PAH clusters are scarcely studied both from a theoretical and an experimental point of view.

We have studied for the first time the interaction of low-energy ions (He^+, He^{2+}, and Xe^{20+}) with cold polycyclic aromatic hydrocarbons clusters of anthracene $[C_{14}H_{10}]_n$ and coronene $[C_{24}H_{12}]_n$. The low-energy ions are delivered by the ARIBE facility of GANIL; they collide with neutral PAH clusters produced in a gas aggregation source. The cationic products of the interaction are mass-over-charge analysed using time-of-flight mass spectrometry.

Experimental results will be presented at the conference with a special emphasis on the specific behaviour of anthracene clusters. They promptly fragment after the interaction with low-energy ions and, very surprisingly, the emitted monomers are much more excited after collisions with highly charged ions than after collisions with ions in low charge states [2].

Acknowledgments: We appreciate support received from the ITS-LEIF project (Grant No. RII3-026015), the Swedish Research Council, and the Danish Council for Independent Research/Natural Science.

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Classical theory of atomic collisions – the first hundred years

P. Grujić

Institute of Physics, POB 57, 11080 Belgrade, Serbia

Classical calculations of the atomic processes started in 1911 with famous Rutherford's evaluation of the differential cross section for α particles scattered on foil atoms. The success of these calculations was soon overshadowed by the rise of Quantum Mechanics in 1925 and its triumphal success in describing processes at the atomic and subatomic levels. It was generally recognized that the classical approach should be inadequate and it was neglected until 1953, when the famous paper by Gregory Wannier appeared, in which the threshold law for the single ionization cross section behaviour by electron impact was derived [1]. All later calculations and experimental studies confirmed the law derived by purely classical theory.

The next step was taken by Ian Percival and collaborators in 60-ies [2], who developed a general classical three-body computer code, which was used by many researchers in evaluating various atomic processes like ionization, excitation, detachment, dissociation etc. Another approach was pursued by Michal Gryzinski from Warsaw, who started a far reaching programme for treating atomic particles and processes as purely classical objects [3]. Though often criticized for overestimating the domain of the classical theory, results of his group were able to match many experimental data. Belgrade group was pursuing the classical approach using both analytical and numerical calculations, studying a number of atomic collisions, in particular near-threshold processes [4]. Riga group, lead by Modris Gailitis contributed considerably to the field, as it was done by Valentin Ostrovsky and coworkers from Sanct Petersbourg, who developed powerful analytical methods within purely classical mechanics [5].

We shall make an overview of these approaches and show some of the remarkable results, which were subsequently confirmed by semiclassical and quantum mechanical calculations, as well as by the experimental evidence. Finally we discuss the theoretical and epistemological background of the classical calculations and explain why these turned out so successful, despite the essentially quantum nature of the atomic and subatomic systems.

Acknowledgments: The work has been supported by Ministry of Science and Technological Development of Republic of Serbia.

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TOPICAL LECTURES

Probing the coherent evolution of wavepackets in high Rydberg states

S. Yoshida[a], C. O. Reinhold[b], J. Burgdorfer[a], B, Wyker[c], S. Ye[c], F. B. Dunning[c]

[a]*Institue for Theoretical Physics, Vienna University of Technology, Austria, EU*
[b]*Physics Division, Oak Ridge National Laboratory, Tennessee, USA*
[c]*Department of Physics and Astronomy and the Rice Quantum Institute, Rice University, Texas, USA*

A wavepacket is a coherent superposition of nondegenerate stationary states and thus evolves in time. With properly chosen complex expansion coefficients in the superposition, a wave packet forms a spatially localized state whose average motion follows the classical dynamical equation. With recent technological advances it is possible to experimentally control expansion coefficients and design wavepackets with different spatial properties. The stored information, i.e. the amplitudes and phases of the coefficients, can be extracted by monitoring the time evolution of the wavepacket. We demonstrate a few examples of such control and probe protocols.

Our control scheme employs a static electric field applied for a finite duration. Even such a simple control field allows to manipulate the properties of wavepackets in great detail. An electric dipole of a Rydberg atom precesses about an electric field. As this resembles the dynamics of a spin in a magnetic field, protocols known from NMR, such as spin echo, can be applied to Rydberg wavepackets. Echoes of a Rydberg dipole can be achieved by a reversal of the Stark precession to recover the initial wavepacket and the reduced amount of echoes serves as a measure of the irreversibility, i.e. decoherence induced in the system [1].

During the dipole precession, the angular momentum l also evolves periodically in time. By turning off the static field, therefore, the evolution of l stops and a wave packet with varying eccentricity can be generated. By maximizing l~n, it is possible to generate circular wavepackets mimicking the dynamics of Bohr model of the atom (Fig.1) [2]. As the orbital frequency E_{n+1}-E_n = n^{-3} depends on n, however, the localized state can be observed only for a limited duration due to the dephasing of different n components. When only a few discrete n levels are involved in the superposition, the wave packet exhibits a series of collapses and revivals. Revivals can be observed by a pump-probe scheme and are useful to extract the information on the complex coefficients of the superposition [3].

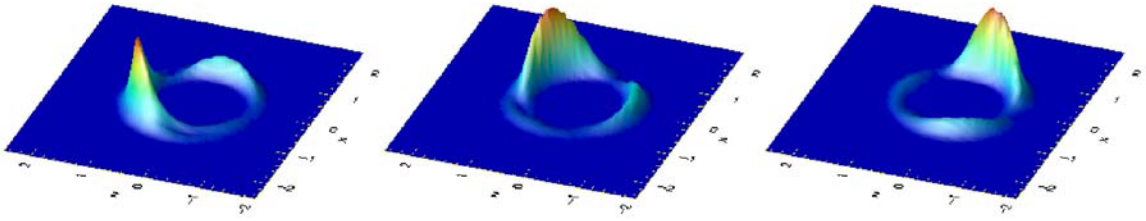

Fig.1. Time evolution of a wavepacket (n~60) traveling along a circular orbit

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Quantum interferences in atomic ionization by short laser pusles

D. G. Arbó

Institute for Astronomy and Space Physics, IAFE (FCEN UBA-Conicet), CC67, Suc. 28 (1428) Buenos Aires, Argentina

Electrons are emitted by tunneling through the potential barrier formed by the combination of the atomic potential and the external strong field. Tunneling occurs within each optical cycle predominantly around the maxima of the absolute value of the electric field [1]. After detachment from the atom, direct electrons can escape without being strongly affected by the residual core potential. Recently, diffraction fringes have been experimentally observed in photoionization of He atoms and photodetachment in F^- ions [2,3], for example.

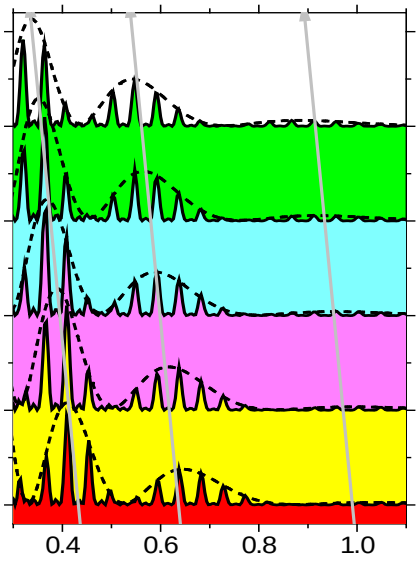

Fig.1. Photoelectron spectra for different values of the nuclear charge Z_T = 0, 0.25, 0.5, 0.75, and 1, calculated within the CVA for a four-cycle pulse (solid line) and a one-and-half cycle (dashed line) with peak electric field F_0 = 0.0675 and frequency ω = 0.0456.

In the talk, different aspects of interference processes in atomic ionization by short laser pulses will be presented. The complex interference pattern observed for the full solution of the time-dependent Schrödinger equation is unraveled in terms of diffraction at a grating in the time domain. The interplay between *intracycle* and *intercycle* interferences will be identified within a semiclassical description of above-threshold ionization, which remains unchanged in the presence of the long range potential of the remaining ion [4,5].

In Fig.1 it can be observed the photoelectron spectra of a hydrogen atom subject to a four-cycle pulse for different values of the nuclear charge Z_T. The multiphoton peaks stemming from *intercycle* interference are modulated by the *intracycle* pattern resulting from the photoelectron spectra of a one-and-half cycle. The shift of the *intracycle* interference pattern towards lower energies as Z_T increases shows the effect of the remnant Coulomb potential of the nucleus. Calculations of Fig. 1 were performed within the Coulomb-Volkov approximation [5].

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Photofragmentation of organic molecules of biological interest

P. Bolognesi, P. O'Keeffe and L. Avaldi

CNR-Istituto di Metodologie Inorganiche e dei Plasmi, Area della Ricerca di Roma 1, Monterotondo, Italy

Soft and hard X-ray exposure causes dramatic effects on living organisms, producing damage, which lead to alterations, malfunctioning and even mutations and cellular death [1]. There is nowadays substantial evidence that macroscopic damage may be initiated at the microscopic scale of the DNA chain, due to significant energy deposition either in the DNA constituents or in its neighbouring molecules. On the other hand, the same pathogenic effects of X-ray radiation are used in radiotherapy for cancer treatment, via the use of properly designed radiosensitisers aiming at a more selective and amplified damage of the tumour rather than healthy cells [2].

The understanding of the interaction between radiation and pyrimidine and halogenated pyrimidines (figure 1) as well as the characterization of the electronic structure of these molecules play an important role in this context. Pyrimidine is the building block of cytosine, thymine and uracil DNA/RNA bases, while the halopyrimidines represent an important class of prototype radiosensitisers, such as for example the bromo- or iodo-deoxyuridine (UdR) or the 5-fluorouracil (5-FU) [3].

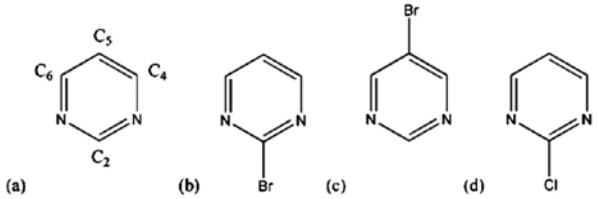

Figure 1. Schematic representation of the pyrimidine molecule (a) and some halogenated pyrimidines (b-d). These molecules are selected with the purpose of investigating the effect of the halogenation on the pyrimidine ring as function of the halogen atom (chlorine/bromine) or atomic site of halogenation (2/5).

Among the physical mechanisms proposed to explain the radiosensitising effect of halogenated pyrimidines, inner shell excitation/ionization are considered among the primary sources of the electron and/or the responsible for the enhanced and selective molecular fragmentation induced in the radiosensitiser rather than on the unsubstituted molecule.

Our works [4-7] aim to provide an extensive characterisation and understanding of the behaviour of the pyrimidine molecule exposed to soft X-ray radiation.

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Excitation reactions studied by electron induced fluorescence method

J. Országh, M. Danko, A. Ribar, Š. Matejčík

Department of Experimental Physics, Comenius University, Mlynská dolina F-2, Bratislava, Slovakia, e-mail: orszagh@fmph.uniba.sk

Studying all kinds of elementary processes induced by low energy electrons seems to be a very current topic nowadays not only in the field of experiment but in modelling as well [1], [2]. An important one from this group of processes is excitation of a molecule by electron impact and subsequent radiative deexcitation. Such series of processes is usually called electron induced fluorescence (EIF).

The scheme of apparatus we use to study the EIF processes is shown in the figure 1. The electron beam of approximately 90 nA produced by trochoidal electron monochromator is colliding with molecular beam in the reaction chamber. The pressure of studied gas in the chamber is in the range of $1x10^{-4}$mbar. The photons produced in this region are collected by system of lenses and focused onto the entrance slit of an optical monochromator. Then they are detected at the exit of monochromator by highly sensitive photomultiplier.

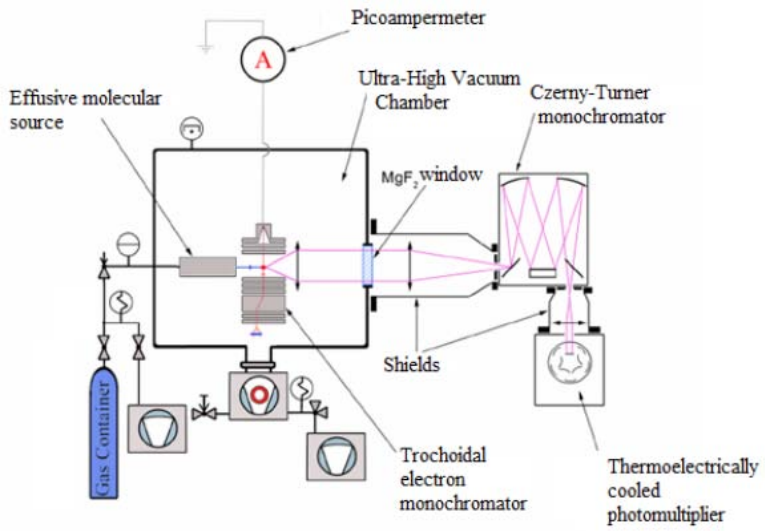

Fig.1. The crossed-beams experimental apparatus used for studying electron/molecular collisions by EIF method.

In our experiments we have focused on observing the first negative system and second positive system of nitrogen and on EIF of methane molecule. We have measured the spectra of these systems and relative cross-sections of many transition processes.

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Differential cross sections of some noble atoms studied by fast electron impact and inelastic X-ray scattering

Lin-Fan Zhu* and Ya-Wei Liu

Hefei National Laboratory for Physical Sciences at Microscale, Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui, 230026, P. R. China
** e-mail: lfzhu@ustc.edu.cn*

According to the Bethe-Inokuti theory [1,2], the differential cross sections (DCSs) of the fast electron scattering (FES) can be described by:

$$\frac{d\sigma_n}{d\Omega} = \frac{2}{E_n}\frac{p_a}{p_0}\frac{1}{K^2}f(E_n, K^2),$$

where $f(E_n,K^2)$ is the generalized oscillator strength (GOS) defined as

$$f(E_n, K^2) = \frac{2E_n}{K^2}\left|\langle\Psi_n|\sum_{j=1}^{N} e^{i\vec{K}\cdot\vec{r_j}}|\Psi_0\rangle\right|^2.$$

$f(E_n,K^2)$ provides a comprehensive description of the excitations, since it reveals the momentum distribution character related to the wavefunctions of the initial and final states ($|\Psi_0\rangle$ and $|\Psi_n\rangle$) [1, 2]. Very recently, the inelastic x-ray scattering (IXS) were introduced to measure the structures of atoms and molecules [3, 4, 5], i.e., the DCSs for the excitations of atoms or molecules by IXS can be represented by:

$$\frac{d\sigma_n^r}{d\Omega} = r_0^2\frac{\omega_f}{\omega_i}|\vec{\epsilon_i}\cdot\vec{\epsilon_f^*}|^2\zeta(\vec{q},\omega_n),$$

herein

$$\zeta(\vec{q},\omega_n) = \left|\langle\Psi_n|\sum_{j=1}^{N} e^{i\vec{q}\cdot\vec{r_j}}|\Psi_0\rangle\right|^2.$$

The symbols in above formulae have their common meanings while $\vec{K}$ and $\vec{q}$ are the momentum transfer in the above two methods.

It can be seen from the above formulae that the structure of atom or molecule can be determined by either FES or IXS, i.e., the wave functions in the momentum space can be explored.

Using the FES and IXS, the DCSs, GOSs and $\zeta(\vec{q},\omega_n)$ for the valence-shell excitations of some noble atoms were measured at an electron energy of 2500 eV and a photon energy of about 10 keV [3, 5, 6]. The good agreement of the $\zeta(\vec{q},\omega_n)$ for helium measured by FES hand IXS elucidates the intrinsic connection between IXS and fast electron scattering, while the difference for the results of neon shows that the contribution from the higherorder Born term may be important for FES with the heavier target. It is also found

that the GOS's for the pair of transitions, which are formed by the same electronic configuration through the intrachannel interaction such as $(n-1)p^5ns[3/2]_1$ and $(n-1)p^5ns'[1/2]_1$ of Ne (n=3), Ar (n=4), and Kr (n=5), are nearly parallel. The possible reason has been discussed.

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Cross sections for elastic electron scattering from iodine

M. J. Brunger[a], L. R. Hargreaves[a], D. B. Jones[a], R. Murrie[a], J. R. Brunton[a], O. Zatsarinny[b], K. Bartschat[b], G. García[c], F. Blanco[d], M. Hoshino[e], S. J. Buckman[f]

[a]*CAMS, CaPS, Flinders University, Adelaide, S.A., Australia*
[b]*Dept. of Physics and Astronomy, Drake University, Des Moines, Iowa, USA*
[c]*IFF, CSIC, Madrid, Spain*
[d]*Atomic, Molecular and Nuclear Physics Dept., Universidad Complutense, Madrid, Spain*
[e]*Dept. of Materials and Life Sciences, Sophia University, Tokyo, Japan*
[f]*CAMS, RSPE, Australian National University, Canberra, ACT, Australia*

Results from a joint experimental and theoretical study of elastic electron scattering from atomic iodine will be described. The experimental results were determined with a unique scattering apparatus [1,2] by subtracting known cross sections from the measured data obtained with a pyrolyzed mixed beam containing a variety of atomic and molecular species. The calculations were performed using both a fully relativistic Dirac B-spline R-matrix (close-coupling) method (BSR) [3] and an optical model potential (OMP) approach [4]. Given the difficulty of this problem, the agreement between the two sets of theoretical predictions and the experimental data for the angle-differential and angle-integrated elastic cross sections at 40 eV and 50 eV is remarkably good [5].

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On deviations from theory of electron-atom elastic scattering cross sections

R. Moreh[a] and D. Nemirovsky[b]

[a]*Physics Department, Ben-Gurion University of the Negev, Beer-Sheva, 84105, Israel*
[b]*Sami Shamoon College of Engineering, Beer-Sheva, 84100, Israel*

In some recent studies it is claimed that the electron elastic scattering intensities at keV energies from atoms and molecules at high momentum transfers do not conform to the Rutherford relation. Huge reductions in the ratios of the electron scattering intensities were reported in the following binary gas mixtures: H_2/D_2, H_2/He, H_2/Ar, D_2/Ar and He/Ar where the intensities from the light partners were found to be lower than the heavier ones by: 30(3)%, 48(6)%, 63(6)%, 45(5)% and 35(8)% respectively [1,2]. It was stated that a quantum mechanical treatment of this scattering process in the framework of the Born approximation could not yield an explanation for the above observation [1].

Of particular interest in the above is the strong reduction in the H-scattering intensity relative to D in H_2/D_2 where the deviations were attributed [2] to short lived quantum entanglement of the two protons in H_2. Similar intensity reductions were reported in samples of solid polymers [3] where the electron scattering intensity from H was compared to that of C.

Here a critical examination of the above reports will be given with the conclusion that the origin of all above deviations is very likely instrumental [4] and not due to any real deviation from the Rutherford formula.

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Spatially resolved transport properties for electrons in gases: Definition, interpretation, and calculation

S. Dujko[a,b], R.D. White[b], Z.M. Raspopović[a] and Z.Lj. Petrović[a]

[a]*Institute of Physics, University of Belgrade, Pregrevica 118, P.O. Box 68, 11080 Belgrade, Serbia*
[b]*ARC Centre for Antimatter-Matter Studies, School of Engineering and Physical Sciences, James Cook University, Townsville 4810, Australia*

Comparison of experimental and theoretical transport data for electrons in neutral gases in varying configuration of electric and magnetic fields provides a rigorous test of electron scattering cross sections. However, the definition, interpretation and way of calculation of transport data are based upon the method of swarm observation. A multi term theory for solving the Boltzmann equation [1] and Monte Carlo simulation technique [2] are reviewed and results of calculations for swarms under hydrodynamic conditions and for those under steady-state Townsend (SST) non-hydrodynamic conditions in certain model and real gases are discussed from a viewpoint how to establish connection between these two sets of data when non-conservative collisions are operative. Two additional fundamental issues: (1) what is the role of elastic, inelastic and non-conservative collisions on the spatial evolution of an electron swarm, and (2) how magnetic fields affect the spatial variations of various transport properties, are discussed on the basis of knowledge attained in the past decade [3,4,5]. A distinctively non-local behavior of spatially resolved transport properties is observed under the SST conditions. It is illustrated that both the magnetic field strength and angle between the electric and magnetic fields have an ability to control the relaxation process: in general, these parameters can be used to enhance or suppress the oscillatory features in the relaxation profiles of various transport properties. Under the hydrodynamic conditions, however, it is found that the full spatial relaxation is achieved under conditions when diffusion fluxes due to gradients in electron number density are much less than corresponding drift due to the electric field force. It is shown that independent of the presence of the magnetic field, the spatial density profile of the swarm relax to a Gaussian profile after a sufficient time while the average energy and/or velocity have the characteristic slope along the swarm. The transient spatial profiles of the density and energy distribution function under both hydrodynamic and non-hydrodynamic conditions demonstrate an initial periodic structure of similar physical origin to those found in the Franck-Hertz experiment.

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Positron scattering from krypton

J. P. Sullivan

Centre for Antimatter-Matter Studies, Research School of Physics and Engineering, Australian National University

Accurate measurements of low-energy positron scattering have long been very difficult, due to low positron beam currents as well as beam energy spreads of typically 0.5 eV or more. The recent development of the Surko positron trap and beam system has made available low energy positron beams of a much higher intensity and energy resolution than has previously been possible [1]. These beams are confined using strong magnetic fields of 500 gauss or more, resulting in the development of new techniques to make measurements of scattering cross sections. This has meant that a new range of measurements are now possible for positron scattering processes, at a much higher precision and accuracy than earlier experiments [2].

At the Australian National University, we have constructed a low energy positron scattering experiment to take advantage of these new developments, and we have developed a broad experimental program in low energy positron scattering. Our positron beam has a typical energy resolution of 60 meV and is tuneable from <1 eV to 200 eV. The pulsed beam is directed through a gas cell containing the target gas of choice, and then energy analysed after the scattering to extract information about the scattering processes which take place. One of the strengths of the technique is that the absolute normalisation relies only on the measurement of the scattering length and the pressure of target gas in the cell, both quantities that are easily measured to a high degree of accuracy [3].

Part of our experimental program concentrates on making benchmark measurements of positron scattering, and includes scattering from a range of noble gas targets, amongst others. Previous work has concentrated on helium [4-6], but recently measurements have been extended to cover the noble gases up to Xe [7].

Previous measurements of positron scattering in krypton have been limited, for the most part, to grand total cross sections, with some data also available for ionisation and positronium formation. Relative measurements of the differential scattering cross section have also been made. In all cases, there is a lack of agreement on the absolute value of the cross sections, and in some cases, the shape. In this paper, I will present a brief description of the experimental apparatus and analysis techniques, along with recent measurements of the grand total, positronium formation and differential elastic cross sections for positron scattering from krypton. Data will be compared to previous experimental and theoretical data, and progress towards establishing a set of benchmark cross sections for positron scattering from krypton will be discussed.

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Resonant inelastic collisions of electrons with diatomic molecules

K. Houfek[a], M. Čížek[a], J. Horáček[a]

[a]*Institute of Theoretical Physics, Faculty of Mathematics and Physics, Charles University in Prague V Holešovičkách 2, 180 00 Praha 8, Czech Republic*

In our contribution we give a review of results of the nonlocal resonance theory [1] which has been successfully used for treating the nuclear dynamics of low-energy electron collisions with diatomic molecules over several three decades. We focus on the explanation of various structures such as threshold peaks, oscillations below the dissociative attachment threshold, or outer-well resonances observed in the cross sections of vibrational excitation and dissociative electron attachment to hydrogen molecule and hydrogen halides.

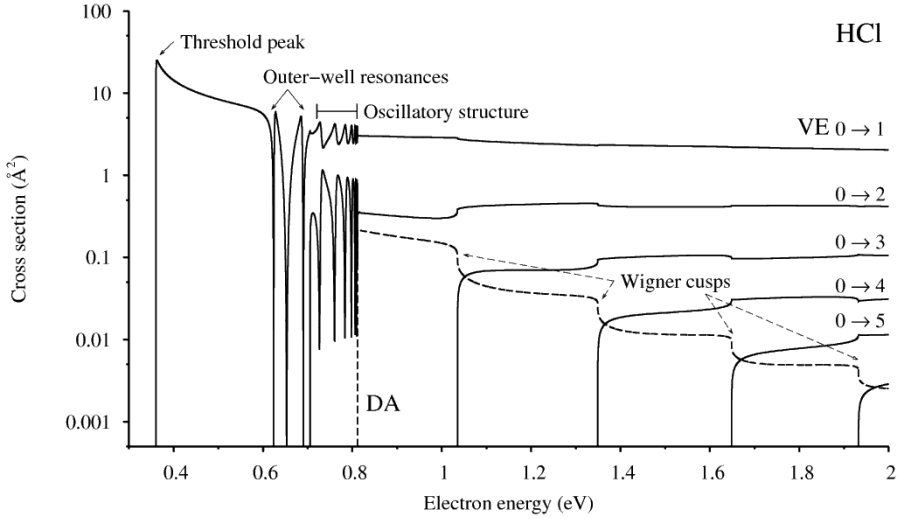

Fig. 1. Examples of structures in the calculated integral cross section of vibrational excitation and dissociative attachment for the molecule HCl up to 2 eV. The results of the nonlocal resonance model of [2].

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Electron driven processes in biomolecules

J. Kopyra[a], H. Abdoul-Carime[b] and E. Illenberger[c]

[a]*Chemistry Department, University in Siedlce, 3 Maja 54, 08-110 Siedlce, Poland*
[b]*Institut de Physique Nucléaire de Lyon, Université Lyon 1, Villeurbanne, CNRS/IN2P3, UMR5822, Université de Lyon, F-69003, Lyon, France*
[c]*Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universitaet Berlin, Takustrasse 3, D-14195 Berlin, Germany*

Electronic mail: kopyra@uph.edu.pl

Chemistry induced by electrons drive plenty of the important processes in radiation chemistry, nanolithography and other technological applications, e.g., stability of waste repositories, gas-phase dielectrics.

It is by now well known that low energy electrons, the secondary species in the interaction of ionizing radiations with matter, efficiently produce structural and chemical modifications in a biological medium. These secondary electrons with a kinetic energy distribution up to 20 eV [1] are created in numbers of $5x10^4$ per MeV of deposited energy [2] that makes them the most abundant radiolytic species.

Recent years have witnessed a remarkable growth in the scientific interest in studying the low energy electron interactions with biomolecules. Among them a number of publications have been devoted to nucleic acids, proteins and the sub-units of proteins, i.e., amino acids [3-5].

In this contribution we will present the results of dissociative electron attachment DEA to simple gas phase amino acids and more complex dipeptide. We will discuss the main differences in electron attachment to amino acids that adopt a canonical or zwitterionic structure in the gas phase. The main observation is that both canonical as well as zwitterionic amino acids attach electrons purely dissociatively. Like in many other biologically relevant molecules the most abundant fragment anion that arise from former structure is the closed shell $(M-H)^-$ anion which is formed from transient precursor anion by the loss of a neutral hydrogen atom. While canonical amino acids form resonances in the energy range 0-12 eV, in the case of zwitterionic Glycine-Betaine [3] resonances only appear in the restricted electron energy range 0-2 eV. This is due to the different mechanism in the formation of the transient negative ion TNI. While in the case of canonical molecules the TNI is formed via shape resonances (at low energy) and core excited resonances (at energy greater then 4 eV) in the case of zwitterionic amino acids TNI formation is mediated by the extremely high dipole moment of 11.5 D [6].

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Photoionization and photodetachment study of trapped biopolymer ions in the gas phase

A. Giuliani[a,b], A. R. Milosavljević[c], C. Nicolas[a], M. Réfrégiers[a], L. Nahon[a]

[a]*Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, BP 48, 91192 Gif-sur-Yvette, France*
[b]*Cepia, Institut National de la Recherche Agronomique (INRA), BP 71627, 44316 Nantes Cedex 3,*
[c]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

Although infrared gas phase spectroscopy is routinely performed at free electron laser facilities [1,2], the use of synchrotron radiation for spectroscopy of trapped ions is still in its infancy. Few couplings of ion traps with monochromatized light have been reported. A Penning trap was used for atomic ion ionization in the XUV [3]. Soon after, a linear ion trap was used for mass selected inner shell spectroscopy on cluster ions [4]. Recently a Paul trap allowed peptide ions to be irradiated in the VUV prior to time of flight mass analysis [5]. Our group has coupled a commercial linear ion trap LTQ XL from Thermo Scientific with the DESIRS beamline at the SOLEIL synchrotron radiation facility [6,7].

The coupling of ion trap fitted with electrospray ion sources with synchrotron radiation in the UV and VUV opens a very interesting field in ion spectroscopy. Indeed, thanks to the softness of electrospray ionization [8], new targets that were previously not vaporizable by other means may now be studied in the gas phase. This is for example the case for non-covalent assemblies. Moreover, the study of isolated species in the gas phase allows accessing spectral regions for the first time. Indeed, the opacity of the solvents and of the cuvettes and sample holders is not a barrier anymore. In addition, this kind of spectroscopy is performed on mass to charge ratio selected species, which brings new possibilities as compared to neutral targets where average properties of ensembles are measured.

Submitting a particular ion to irradiation may result in two main phenomena: fragmentation and photoionization or photodetachment. The particular features of stored ion spectroscopy will be illustrated for poly-protonated and poly-deprotonated ions of biopolymers in the VUV range. The application in structural analysis of biomolecule will be discussed.

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Absolute differential cross sections for electron scattering from building blocks of biopolymers

A. R. Milosavljević[a], F. Blanco[b], J. B. Maljković[a], G. García[c] and B. P. Marinković[a]

[a]*Laboratory for Atomic Collision Processes, Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[b]*Departamento de Física Atómica Molecular y Nuclear, Facultad de Ciencias Físicas, Universidad Complutense, Avda. Complutense s/n, E-28040 Madrid, Spain*
[c]*Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 121, 28006 Madrid, Spain*

Beside a fundamental interest to investigate processes of electron interaction with different molecular systems and test corresponding available theoretical models, the investigation of electron interaction with the molecules representing building blocks of large biopolymers (DNA, RNA, proteins) has been dominantly motivated in recent years by the research on radiation damage in biomolecular systems. The primary high-energy ionizing particles produces on its track a large number of secondary low-energy electrons, which carry most of the energy deposited in the tissue and may play an important role in the final radiation damage [1].

In recent years, we have reported both experimental and theoretical absolute differential cross sections (DCSs) for electron interaction with several different molecules representing building blocks of DNA [2-5]. The present experimental procedure includes three independent measurements, namely: 1) relative DCSs measured at a fixed incident electron energy as a function of scattering angle, 2) relative DCSs measured at a fixed scattering angle as a function of the incident electron energy and 3) absolute DCSs obtained at specific scattering angle and incident energy by applying relative flow technique, with Ar of Kr as reference gases. All these independent measurements make up a consistent set of absolute DCSs for a specific target, which is finally compared to the theoretical results. The calculations of molecular cross sections are based on a corrected form of the independent-atom method, known as the SCAR (Screen Corrected Additivity Rule) procedure and using an improved quasifree absorption model. For all treated molecular targets, a very good agreement between the experimental and theoretical results has been obtained.

The present contribution discusses previously obtained results, comparison between the experiment and the theory, as well as different target molecules. The difficulties and drawbacks of the experimental procedure are particularly elaborated. Additionally, some preliminary results for molecules representing the smallest systems containing the peptide bond, which links amino acids in protein chains, will be reported, as well.

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Thermo-mechanical impact on biomolecules induced by ion beams propagating in biological medium as seen from molecular dynamics simulations

A.V. Yakubovich[a], E. Surdutovich[b], A.V. Solov'yov[a]

[a] *Frankfurt Institute for Advanced Studies/Goethe University, Frankfurt am Main, Germany*
[b] *Department of Physics, Oakland University, Rochester, Michigan 48309, USA*

The structural nano-scale transformations in finite molecular systems, i.e. the transition from a stable 3D molecular structure to a random coil state and vice versa (also known as (un)folding process) occur in many different complex molecular systems and in nano objects, such as polypeptides, proteins, polymers, DNA, fullerenes, nanotubes, etc. [1].

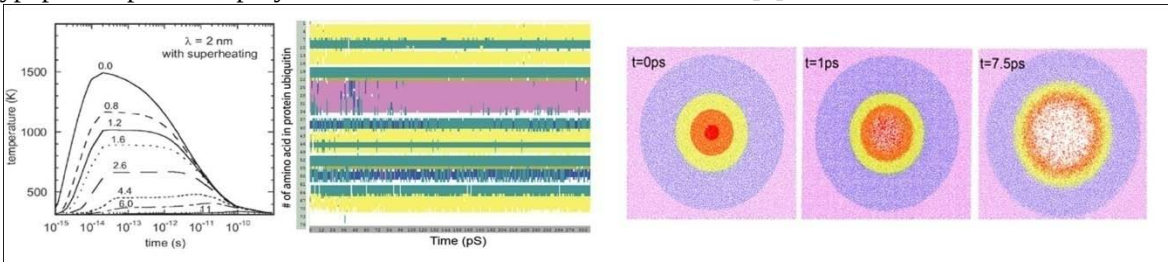

Fig.1. Left: Energy deposition in eV/atom on the molecular subsystem versus time assuming a superheating scenario. The calculations have been performed for C ions at 0.5 MeV/u with an electronic energy loss of 0.91 keV/nm [2]. Center: The dependence of the secondary structure of protein ubiquitin on time obtained using molecular dynamics simulations. The protein is exposed to the heat spike produced by the propagation of an energetic particle. Prominent disturbance of the secondary structure is observed during first 100 ps after the propagation of a particle [3]. Right: The snapshots of molecular dynamics simulation of the heat spike. Only oxygen atoms of water molecules are shown. Three images correspond to 0, 1 and 7.5 ps after ion's passage, respectively. By violet, yellow, orange and red colors are shown water molecules initially located 10nm, 5nm, 3nm and 1nm away from the ion's track, respectively. From the left figure it is seen the formation of a strongly vacuated cylinder with radius of ~ 3-5*nm* at 7*:*5*ps* after ion's passage.

We focus on the transformations in biomolecules caused by the near passage of energetic particles – carbon ions. In particular we consider the possibility of the creation of the shock waves in the vicinity of the ion tracks. We demonstrate that at the initial stages after ion's passage the shock wave is so strong that it can contribute to the DNA and protein damage due to large pressure gradients developed at the distances of a few nanometers from the ionic tracks. This novel mechanism of damage of biomolecules provides an important contribution to the cumulative biodamage caused by low-energy secondary electrons, holes and free radicals.

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Electron-impact and thermal fragmentation of the amino acid molecules: mechanisms and structure of the molecules

J. Tamuliene[a], L.G. Romanova[b], V.S. Vukstich[b], A.V. Snegursky[b]

[a] *Vilnius University, Institute of Theoretical Physics and Astronomy, 12 A. Goštauto str., 01108, Vilnius, Lithuania*
[b] *Institute of Electron Physics, Ukr. Nat. Acad. Sci., 21 Universitetska str., 88017 Uzhgorod, Ukraine*

The studies of the damages in biological systems, including amino acids, resulted from the influence of ionizing radiation, are the hot topic of a series of investigations within last decades [1]. The majority of the above damages is usually due not to the primary high-energy radiation but results from the effect of the secondary low-energy charged particles produced in the course of ionization. Moreover, the problem of thermal degradation of the initial molecules should also not be avoided. Amino acids play a central role both as building blocks of proteins and as intermediates in metabolic processes. Proteins do not only catalyze the most of the reactions in living cells but also control all cellular processes.

Here we report on the results of the mass-spectrometric studies of the amino acids ionic fragment production due to the low-energy electron impact accompanied by the theoretical determination of the possible mechanisms of the electron impact-induced fragmentation and thermal degradation of the initial molecules. The details of the present experiment using the magnetic mass-spectrometer combined with the crossed electron-molecular beam technique could be found elsewhere [2]. Our apparatus is capable of studying the ionic fragments within the 1–720 a.m.u. mass range with high sensitivity (~10^{-16} A) and mass resolution (m/Δm=1100). The beam of the molecules under study was formed by an effusion source with a resistively heated oven providing the target molecule concentrations of about 10^{10} cm^{-3}. The operating temperature of the molecular beam source was varied up to 150°C allowing the optimal conditions of beam generation to be chosen. The main emphasis has been given to the electron-impact fragmentation of the glycine and methionine molecules including the analysis of the thermal degradation issues.

The structure of the molecules and their fragments has been studied using the generalized gradient approximation for the exchange-correlation potential in the density functional theory [3] as it is described by the Becke's three-parameter hybrid functional, using the non-local correlation provided by Lee, Yang, and Parr. The cc-pVTZ basis set has been used as well. The structure of the molecules and their fragments under study has been optimized globally without any symmetry constraint. Additionally, the vibration spectra were evaluated to predict the possible elongation bonds and angles in order to analyze the possible fragments produced under electron impact.

Production of the double-charged CH_2NHCO^{++} glycine molecule fragment was observed for the first time. An assumption about the mechanism of production of this fragment by a simultaneous elimination of two electrons and the water molecule is confirmed by theoretical calculations according to which the least energy consumption corresponds to the C–H bond break being accompanied by the neutral (OH + H) fragments yield.

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Title of the hard X-ray polarimetry in energetic ion-atom collisions

G. Weber[a,b], H. Bräuning[b], S. Fritzsche[b,c], S. Hess[b], R. Märtin[b,d], R. Reuschl[b,e], U. Spillmann[b], A. Surzhykov[b,c], D. F. A. Winters[b], and Th. Stöhlker[a,b,d]

[a] *Helmholtz-Institut Jena, Helmholtzweg 4, 07743 Jena, Germany*
[b] *GSI, Planckstrasse 1, 64291 Darmstadt, Germany*
[c] *Department of Physics, University of Oulu, 90014 Oulu, Finland*
[d] *Physikalisches Institut, Ruprecht-Karls-Universität, Philosophenweg 12, 69120 Heidelberg, Germany*
[e] *ExtreMe Matter Institute EMMI, Planckstrasse 1, 64291 Darmstadt, Germany*

Studies of the polarization of hard x-rays emitted in energetic heavy-ion atom collisions provide detailed information of the collision dynamics as well as of the atomic structure at high-Z [1]. Moreover, hard x-ray polarimetry also opens a route for polarization diagnosis of spin-polarized ion and electron beams as are discussed for future PNC experiments [2,3]. However, due to the lack of efficient polarimeters previous studies of the radiation stemming from highly-charged ions were mainly restricted to measurements of the spectral and angular distribution. Owing to recent progress in the development of highly segmented solid-state detectors, a novel type of polarimeter for the hard x-ray regime has become available. Applied as Compton polarimeters, two-dimensional position-sensitive x-ray detectors now allow for precise and efficient measurements of photon linear polarization properties in the energy region between 70 and a few 100 keV [4,5,6]. First measurements performed at the ESR storage ring at GSI [4,6,7] and at the polarized electron source SPIN at the TU Darmstadt [8] will be presented.

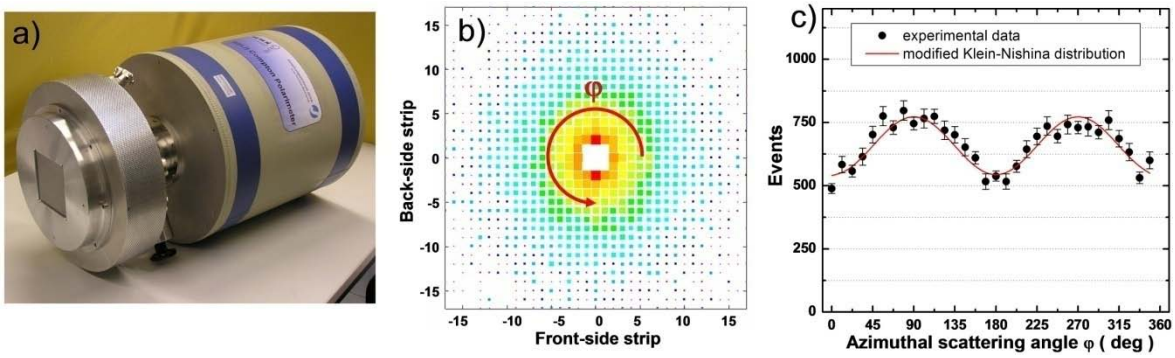

Fig.1. a) Si(Li) Compton polarimeter dedicated for hard x-ray polarimetry [5]; b) position distribution of the Compton scattered photons inside the detector crystal; c) projection of the scatter distribution to the azimuthal scattering angle φ. The red line results from a least-squares adjustment of the Klein-Nishina equation to the experimental data with the degree of polarization treated as a free parameter. In the present case the Lyman-□ transition of U^{91+} was studied and the scatter distribution corresponds to a linear polarization of about 23 % [6].

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Wake effect in the polarization of graphene by slowly moving charges

I. Radović[a], V. Borka Jovanović[a], D. Borka[a], Z.L. Mišković[b]

[a]*VINČA Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia*
[b]*Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, Canada, N2L 3G1*

There has been a growth of interest in recent years to study the low-energy plasmon excitations in graphene by means of high-resolution electron energy loss spectroscopy (HREELS), which uses reflection of electrons under oblique incidence upon supported graphene at energies on the order of 10 eV [1]. Under such conditions, the parallel component of the electron velocity may give rise to a wake pattern in the dynamic polarization of the target surface [2]. Similarly, the wake effect also arises during grazing scattering of low-energy ions from surfaces [2], and it was observed in the emission of convoy electrons [3]. Therefore, it is of interest to investigate the occurrence of a wake in graphene due to slow charges moving on a parallel trajectory at the speed on the order of the Fermi speed of graphene's π-electron band $v_F \approx c/300$, where c is speed of light in vacuum.

In this work, we study the dynamic polarization of doped graphene by an external charge, assuming that equilibrium density of charge carriers can be controlled by applying a gate potential. Calculations of the induced number density per unit area of charge carriers in graphene and the total electric potential in the graphene plane, as functions of the position relative to the moving projectile, were performed by means of the polarization function within the random phase approximation (RPA) based on a linear approximation for the π electron bands [4]. Specifically, we investigate the effects of the projectile speed and distance, the equilibrium charge carrier density in graphene, and finite damping rate of plasmons that is included through the use of Mermin's procedure [4]. We are particularly interested in how Landau damping of plasmons due to interband single-particle excitations in graphene affects the wake because such processes are absent in other targets [2,3]. Furthermore, we also explore the effects of supporting substrate on wake patterns in graphene by specifically considering the size of the gap between graphene and the substrate, as well as the influence of surface phonon excitations in a strongly polar substrate such as SiC.

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Channeling of charged particles through carbon nanotubes

D. Borka

Atomic Physics Laboratory (040), Vinča Institute of Nuclear Sciences, University of Belgrade, P. O. Box 522, 11001 Belgrade, Serbia

This investigation contains a theoretical consideration of the process of charge particles channeling through carbon nanotubes. We begin with a very brief summary of the theoretical and experimental results of studying charged particles (electrons and ions) channeling through carbon nanotubes. Then, the process of charged particles channeling is described briefly [1, 2].

We investigate the angular and spatial distributions of charged particles of the MeV energy range after channeling through different types of carbon nanotubes. The angular and spatial distributions of channeled charged particles are generated using a Monte Carlo computer simulation code [1, 2].

We analyze and explain the angular and spatial distributions of transmitted charged particles. Also, we discuss the problems of guiding of charged particle beams by nanotubes and possible applications for creating nanosized charged particle beams to be used in materials science, biology and medicine.

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The effect of temperature on guiding of slow highly charged ions through mesoscopic glass capillaries

R. J. Bereczky[a], G. Kowarik[b], F. Ladinig[b], K. Tőkési[a], and F. Aumayr[b]

[a]*Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), 4001 Debrecen, Hungary*
[b]*Institute of Applied Physics, TU Wien - Vienna University of Technology, 1040 Vienna, Austria*

Since its discovery in 2002 [1], capillary-guiding of charged particles has become an intensively studied field. The basic concept is the transmission of charged particles through insulating nano-sized capillaries under incident angles much larger than the geometrical limitation due to the self-organized formation of charge-patches at the inner wall [2, 3]. Recently, we were able to show the validity of this so-called guiding effect up to a meso- and even macroscopic length-scale of straight glass capillaries [4, 5].

In this work we present first transmission measurements of highly charged ions through a single high aspect ratio glass capillary (length about 1 cm, aspect ratio about 80) made of Duran (borosilicate glass), with a recently developed and built temperature regulated sample holder, which utilizes surrounding copper parts in order to assure a uniform temperature over the sample (see Fig. 1). In order to avoid strong fields and to provide proper symmetry, the outside of the glass tube is graphite-covered. The measurements are carried out using beams of 4.5 keV Ar^{9+} ions produced by the Vienna 14.5 GHz electron cyclotron resonance ion source. Approximately 18 cm behind the entrance of the capillary, a position sensitive detector mainly consisting of a Chevron-type micro-channel-plate and a wedge-and-strip-anode is used to record the transmitted ions.

By changing the temperature of the glass capillary we are able to manipulate the electrical conductivity of the glass by several orders of magnitude and therefore study the effect of conductivity on the build-up and removal of charge patches in the capillary. We found large influence of the glass temperature (i.e. conductivity) on the transmission of ions which can be compensated by adjusting the incident ion flux.

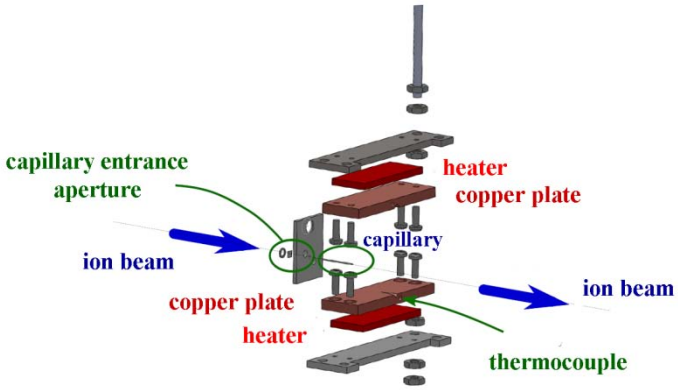

Fig.1. Temperature regulated capillary holder developed in order to study the effect of electrical conductivity on guiding of slow highly charged ions through mesoscopic glass capillaries.

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Laser Raman scattering from biomolecules in nanoparticles-embedded tissue

S. Cintă Pinzaru[a*], A. Falamas[a],C. Dehelean[b]

[a]*Faculty of Physics, Babes-Bolyai University, RO-400084 Cluj-Napoca, Romania*
[*]*simona.cinta@phys.ubbcluj.ro*
[b]*Faculty of Pharmacy, "Victor Babeş" University of Medicine and Pharmacy, Timişoara, Romania*

When laser light is scattered from molecules, most photons are elastically scattered within the so-called Rayleigh effect. However, a small ratio of incident photons (cca.10^{-6}) are inelastic scattered within the Raman effect and the resulted frequencies resemble the Raman spectrum of the given sample. Since the Raman signal is rather weak and there are a lot of poor scattering compounds within the complex samples like bioprobes, new strategies to enhance the signal are required. Among them, surface enhanced Raman scattering (SERS) uses noble metal nanoparticles for the enhancement of the Raman signal, based on the surface plasmon resonance effect [1]. The usually weak Raman scattering signal could be completely quenched when a visible laser line is employed for bioprobe excitation. Quenched fluorescence and greatly enhanced signal could be obtained when Raman scattering takes place on molecules located in the close vicinity of Au or Ag nanoparticles. The SERS effect is mainly employed for the investigation of the molecular species adsorbed on noble metal nanoparticles. Recently, SERS was applied in the study of biological cells and tissue and proved great potential for a wide variety of applications in areas where nucleic acid identification is involved and could lead to the development of detection methods that minimize the time, expense, and variability of preparing samples. [2].

This work is intended to provide the latest results in our group in the field of surface enhanced Raman spectroscopy applied in biomedical field. We demonstrate the possibility to record high quality Raman-enhanced signal from complex biosamples using even visible laser excitation wavelengths. Moreover, employing molecules with high scattering cross section as SERS tags, we were able to record high quality SERS signal from complex biosamples like skin or organs. Prospects on SERS cancer diagnostic have been conducted based on the supposition that Raman scattering signal from altered bioprobe should provide specific spectral fingerprint compared to the normal one. Mice specimens employed in this study were inoculated with B16 melanoma cells and autopsy samples were collected at different stages of malignancy. The Ag nanoparticles-embedded samples were employed to spectroscopic measurements and revealed that the Ag nanoparticles penetrated the tissues and enhanced the signals especially from nucleic acids [2]. These observations proved the fact that SERS is capable of investigating biological systems and of diagnosing the samples at an early stage of malignancy.

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Scattering from biomolecules in helium droplets

S. Denifl[a], F. Ferreira da Silva[a,b], P. Bartl[a], A.M. Ellis[c], T.D. Märk[a], P. Scheier[a]

[a] *Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstrasse 25, A- 6020 Innsbruck, Austria*
[b] *Present address: Departamento de Física, Universidade Nova de Lisboa, Portugal*
[c] *Department of Chemistry, University of Leicester, University Road, Leicester LE1 7RH, UK*

Low energy electrons formed by the interaction of high energy radiation with biological matter are an important species for radiation damage on the molecular level [1]. In the present study we investigated the interaction of electrons with helium droplets doped with biomolecules. Helium nanodroplets are known to be an ideal matrix to form novel agglomerates when atoms or molecules are embedded in the droplet [2]. Due to their low temperature conditions similar to the interstellar medium are also achieved, which allow investigations on astrochemically relevant questions. After the formation of doped droplets they are ionized by inelastic electron scattering (ionization/attachment) and the resulting ions are mass analyzed by various mass spectrometric techniques.

The emergence of homochirality in living systems is not fully explained. A strong chirality preference was reported in clusters of the amino acid serine. We have studied clustering of serine in helium nanodroplets and have observed a profound change in the shape of the serine cluster distribution with decreasing droplet size [3]. Possible explanations for such a pronounced effect on the cluster distribution will be discussed and compared with the previous studies carried out in [3].

Another important question in studying radiation damage on the molecular level is the question of solvent effects, i.e. how fragmentation of an ionized molecule is changed by the possibility of energy transfer into the surrounding solvent? In order to investigate this possibility we embedded the amino acid valine and water molecules in helium droplets and determined the change of the fragmentation pattern upon electron ionization of the doped droplets [4].

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Nanosecond-timescale UV multi-photon ionization of DNA base monomers and hydrated clusters

S. Eden, B. Barc, P. Cahillane, and N.J. Mason

Department of Physics and Astronomy, The Open University, Walton Hall, Milton Keynes, MK7 6AA, UK

The photophysics of DNA and its constituent molecules has attracted considerable research interest for many years. The central aim is to understand the electronic excitation and relaxation pathways that can initiate reactivity and the formation DNA lesions [1]. Information of this kind can lead to improvements in nano-scale models of radiation effects in biological material and thus guide radiotherapy innovations.

Adenine monomers and hydrated complexes have been probed by ns-timescale multi-photon ionization (MPI) time-of-flight mass spectrometry at 223-227 nm. By studying ion production as function of laser fluence on a pulse-by-pulse basis, photon orders were determined for the production of specific ions and cluster ions. For the first time, a photon order of ≥ 1 was observed for adenine monomer ionization. Recent ultrafast studies indicate that the first stages in this process are $^1\pi\pi^*$ excitation followed by internal conversion (IC) on a sub-ps timescale [2]. As 2 photons are energetically sufficient to ionize adenine and photoionization cross sections from highly excited vibrational states are generally low, we expect isomeric transitions to play a significant role in the ns MPI pathway. Further new results include the demonstration that clustering with water not only increases the photon order required for adenine ionization; it also suppresses dissociative ionization as a proportion of total ionization. The photon order for $A^+(H_2O)$ production has been determined for the first time ($\geq 1.8\pm0.2$) and compared with A^+ and AH^+ production ($\geq 2.9\pm0.2$) in ns MPI experiments on $A_m(H_2O)_n$ clusters. We propose that this can be understood in terms of the molecular ions stemming primarily from $^1\pi\pi^*$ excitations followed by IC and complete cluster break-up, whereas $A^+(H_2O)$ may come from $^1\pi\pi^*$ or $^1n\pi^*$ excitations followed by intersystem crossing into ns-lifetime $^3\pi\pi^*$ states of $A(H_2O)_n$ [3,4].

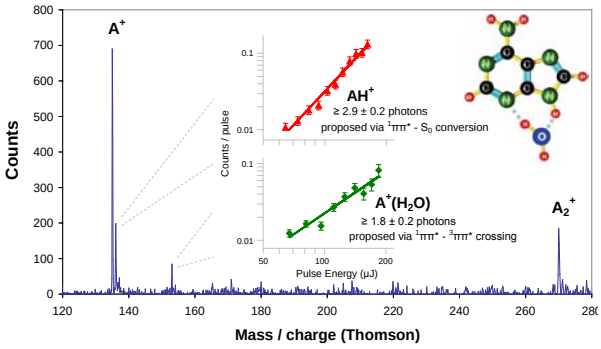

Fig.1. UV MPI (223.8 nm, 2×10^6 Wcm^{-2}) mass spectrum of hydrated adenine. Inserts: pulse energy dependence for AH^+ and $A^+(H_2O)$ production and a schematic of the lowest-energy geometry of $A(H_2O)$ [5].

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Nanostructures formed on various surfaces due to the impact of individual slow highly charged ions

R. Ritter[a,*], G. Kowarik[a], R. A. Wilhelm[b], R. Heller[b], R. Ginzel[c], L. Maunoury[d], M. Toulemonde[d], C. Dufour[d], H. Lebius[d], R. M. Papaléo[e], W. Rupp[f], Q. Shen[g], C. Teichert[g], S. Facsko[b], J. R. Crespo López-Urrutia[c], J. Ullrich[c], and F. Aumayr[a]

[a]*Institute of Applied Physics, TU Wien - Vienna University of Technology, 1040 Vienna, Austria, EU*
[b]*Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany, EU*
[c]*Max-Planck Institut für Kernphysik, 69029 Heidelberg, Germany, EU*
[d]*CIMAP, ENSICAEN, CEA, CNRS, Univ.Caen, 14070 Caen, France, EU*
[e]*Faculty of Physics, Catholic University of Rio Grande do Sul, 90619-900 Porto Alegre, Brazil*
[f]*IMS Nanofabrication AG, 1020 Vienna, Austria, EU*
[g]*Institute of Physics, Montanuniversität Leoben, 8700 Leoben, Austria, EU*

In recent years a variety of materials has been found, which is susceptible to nano-structuring by the impact of slow (keV) highly charged ions (HCI). The nature, appearance and stability of the created structures, however, depend heavily on the properties of the target material and the involved interaction processes and can range from hillocks (CaF_2 [1]), pits (KBr [2], PMMA), caldera-type structures (TiO_2 [3]) to erasable regions of enhanced friction (HOPG [4], mica [5]).

We have systematically studied HCI induced pit formation on poly(methyl metacrylate) (PMMA), a polymer commonly used as a photoresist in the semiconductor industry. Samples were irradiated with Xe ions in charge states q = 12 – 48 and with Bi^{62+} ions. Final impact energies on the surface ranged from 0.35 - 4.0 keV/amu. Intermittent contact mode atomic force microscopy (AFM) investigations of the irradiated samples revealed that each individual ion creates a nano-sized pit above a potential energy threshold of ~ 7.3 keV (Xe^{24+}), above of which the pit-volume increases with the potential energy of the incoming ions, whereas a variation of the kinetic energy of the HCI seems to solely alter the shape of the pit created. A faster ion leaves behind a deeper and slimmer pit compared to a slower ion, while the total volume removed stays approximately the same in both cases. After exposure of the films to a suitable etchant (2-Isopropanol, e.g.), a larger pit volume is found, which is caused mainly by an increase in pit depth and, to a much lesser extent, in pit diameter.

On HOPG, we find nanostructures for all combinations of charge states (Ar^{q+}, q = 9 – 16, Xe^{q+}, q = 13 – 40, 48 and Bi^{62+}) and kinetic energies (0.35 - 3.7 keV/amu) via scanning tunneling microscopy. With the AFM, however, for all but two very high charge states these structures only become visible when operated in lateral force mode. The impact sites can therefore be interpreted as regions of enhanced friction while there is no indication for a topographic surface modification in the lower end of the investigated charge state regime. A first indication of a topographic surface modification could be found only for the two highest charge states employed (Xe^{40+} and Bi^{62+}). In these cases, we find hillock-like structures also by means of intermittent contact mode AFM, where lateral forces are practically eliminated from the measuring process.

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POSTER CONTRIBUTIONS

Intracycle interferences traces in 2D-momentum distribution of atomic photoionization

D. G. Arbó [a], K.L. Ishikawa [b], E. Persson [c] and J. Burgdörfer [c]

[a] *Institute for Astronomy and Space Physics, IAFE (FCEN UBA-Conicet), CC67, Suc. 28 (1428) Buenos Aires, Argentina*
[b] *Photon Science Center, The University of Tokyo, Tokyo 113-8656, Japan*
[c] *Institute for Theoretical Physics, Vienna University of Technology, A-1040 Vienna, Austria*

Interference effects observed in the electron yield of atomic ionization due to the interaction with linearly polarized high intensity laser pulses are studied [1]. The interplay between *intra*- and *intercycle* interferences of electron trajectories leads to modulations in the photoelectron doubly-differential momentum distributions. *Intercycle* interference corresponds to the well-known ATI peaks of the photoelectron spectrum arising from the superposition of wave packets of different optical cycles, whereas *intracycle* interference comes from the coherent superposition of electron wave packets released within the same optical cycle. The latter corresponds to a diffraction grating in the time domain [1,2]. In Fig. 1 we display the two-dimensional momentum distribution calculated by numerically solving the time-dependent Schrödinger equation (lower figure) and by using a calculation based on the Simple Man's Model (upper figure). The *intercycle* interference pattern can be seen as concentric rings, which are modulated by the *intracycle* interference observed as oblique stripes. The *intracycle* interference modulation is independent of the total number of optical cycles involved in the laser pulse and is affected by the long-range nature of the atomic potential.

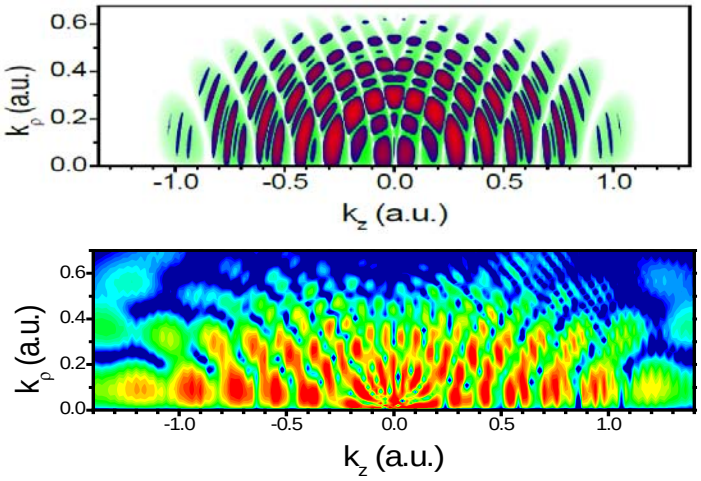

Fig.1. 2D-momentum distribution by a laser of $2x10^{14}$ W/cm^2 and 800 nm. Upper: Semiclassical *intracycle* pattern in green (light grey) and complete (*intra*- and *intercycle*) pattern in blue and red (dark grey). Lower: TDSE calculations.

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Spin effects in nonlinear Compton scattering in a plane-wave laser pulse

M. Boca, V. Dinu, V. Florescu

Centre for Advanced Quantum Physics, University of Bucharest,
PO-Box MG-11, Magurele, RO-077125

Several recent papers are devoted to nonlinear Compton effect, an old subject in the field of the electron interaction with very intense electromagnetic radiation, and to other strong field QED effects that could be detected in the next future [1,2]. We have continued our research [3] on scattering of free electrons on an intense electromagnetic pulse (plane wave with finite extension along the direction of the propagation) in the quantum formalism, in which Volkov solutions are used to describe the electron interacting with the laser field and the interaction with the quantized field describing the emitted photon is treated in the first order perturbation theory.

In the case of a spin 1/2 particle we investigate systematically the effects of the spin of the initial electron and of the laser pulse polarization on the spectrum of the emitted radiation and the distribution of the initial energy. For the case of an electron with well defined initial spin, we discuss the spin flip.

We include a comparison with the scattering process undergone by a spinless particle. The interaction of a spin 0 charged particle with a laser pulse is described in formalism similar to that for the electron, now based on the Gordon-Volkov solutions of the Klein-Gordon equation, valid for the charged particle in an external plane-wave electromagnetic field. The comparison is done with the fully differential cross sections corresponding to an unpolarized incident electron with no detection of the scattered electron spin. Integrating on the electron energy and direction, we obtain also the spectrum and the angular distribution of the emitted radiation and we prove that these distributions, for a spinless and for a spin 1/2 particle, become identical in the classical limit.

The numerical results include both photon and electron differential distributions. We focus on the high intensity regime (intensity of the order of tens of atomic units) and very energetic electrons (Lorentz factor of the order of 10^4 or larger). The differences between the behaviors of a spin 1/2 and a 0 spin particle are displayed in the results of a systematic numerical comparison of the final charged particle and emitted photon cross sections , as function of the initial particle energy and laser intensity. Two collision geometries are considered (head-on collision and 90 degrees collision) , both for circular or linear polarization of the laser field. In all cases we identify the direction in which the probability of detection of the final photon or of the charged particle is maximum.

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Multiphoton excitation in a Γ-type three-level system with generally nondegenerate excited states

D. B. Popović, I. P. Mendaš

Institute of Physics, P.O.Box 57, 11001 Belgrade, Serbia

A study of multiphoton excitation in a Γ-type three-level system with generally nondegenerate excited states is presented. Such systems are formed by the three lowest states in, e.g., hydrogen atom or evenly charged homonuclear diatomic molecular ions under moderate laser intensities. A unitary transformation is introduced for such system, and the transformed Hamiltonian is simplified using Fourier-Bessel expansion. Specifically we considered the case of one dimensional model of evenly charged homo-nuclear diatomic molecular ion A_2^{4+} (A = nitrogen, oxygen or iodine). Obtained results indicate that such approximation is in a good agreement with exact numerical results.

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Propagation of a laser pulse train under electromagnetically induced transparency conditions

G. Buica

Institute for Space Sciences, P.O. Box MG-23, Ro 77125, Bucharest-Magurele, Romania

Electromagnetically induced transparency (EIT) represents a coherent optical nonlinearity which renders a medium transparent over a narrow spectral range within an absorption line. An opaque optical medium can be rendered transparent to a probe field by applying an intense laser field of different frequency. It was theoretically proposed by O.Kocharovskaya and Ya.I.Khanin [1] and it was first experimentally observed in Sr by K.J. Boller et al [2]. We will essentially investigate the space-time dynamics of a train of ultrashort laser pulses in an optical thick absorbing medium under the electromagnetically induced transparency conditions [4-6]. The amplitude equations together with the Maxwell equations which describe the interaction of a three level lambda-type atom with a probe and a coupling laser are numerically solved. We use a laser pulse train with a very short repetition period such that the atom does not have enough time to relax between two consecutive pulses and therefore we expect *new coherent accumulation effects* during the propagation through medium. We analyze how the propagation of the probe laser pulse train into the absorbing medium is modified by varying the parameters of the laser pulse train.

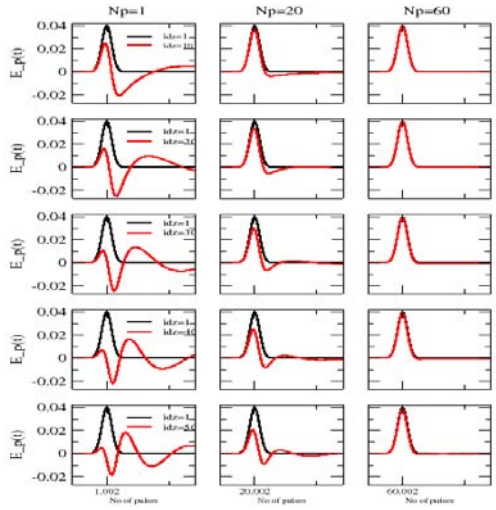

Fig.1. Comparison of the train pulse propagation in a medium for different depths as a function of the number of individual pulses in the train

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Preparing isolated vibrational wave packets by light-induced molecular potentials with chirped laser pulses

M. Vatasescu

Institute for Space Sciences - The National Institute for Laser, Plasma and Radiation Physics
MG-23, RO-77125 Bucharest-Magurele, ROMANIA

Light-pulse shaping has given rise to various possibilities to control quantum processes. One of them is the use of light-induced molecular potentials to direct vibrational dynamics in molecules: laser pulses are used to selectively open and close field-induced avoided crossings, leading to manipulation of the vibrational population [1].

We consider a specific wave packet preparation arising from the control of tunneling in the $0_g^-(6s,6p_{3/2})$ double well potential of Cs_2 molecule with chirped laser pulses. Such a possibility to manipulate the population dynamics in the $0_g^-(6s,6p_{3/2})$ potential effectively appears in a pump-dump scheme designed to form cold molecules by photoassociation of two cold cesium atoms [2,3]. The initial population in the $0_g^-(6s,6p_{3/2})$ double well is a wave packet prepared in the outer well at large interatomic distances (~90 a_0) by a photoassociation step with a first chirped pulse [2], being a superposition of several vibrational states whose energies surround the energy of a tunneling resonance [4]. Our present work is focused on a second chirped pulse, coupling the $0_g^-(6s,6p_{3/2})$ surface with the $a^3\Sigma_u^+(6s,6s)$ one in the zone of the double well barrier (~15 a_0) and creating deeply bound cold molecules in the $a^3\Sigma_u^+(6s,6s)$ state. We explore the parameters choice (intensity, duration, chirp rate and sign) for this second pulse, showing that picoseconds chirped pulses can lead to trapping of population in the inner well in deep vibrational states, out of the resonant tunneling able to transfer it back to the outer well. Then after the pulse a part of the $0_g^-(6s,6p_{3/2})$ wave packet remains stored in the inner well. We analyze the results in terms of light-induced potentials with chirped laser pulses [5] and examine the tunneling dynamics in position and momentum spaces.

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Perturbative solution for analysis of processes in a double-Λ atomic scheme

J. Dimitrijević, D. Arsenović and B. M. Jelenković

Institute of Physics, University of Belgrade, Pregrevica 118 11080 Belgrade Serbia

We solve optical Bloch equations (OBEs) for atomic scheme that consists of four atomic levels which constitute double-lambda (Λ) configuration i.e., two Λ systems sharing the same two ground levels. Double-Λ atomic scheme has being used as a basis for many interesting applications in atomic physics and nonlinear optics. It has been studied in the context of four-wave mixing [1], electromagnetically induced transparency [2], lasers without inversion [3] etc. More recently, it has been shown to be interesting media for phenomena like slow and stored light [4], quantum mechanical entanglement of two beams of light [5] and squeezed light [6].

Typically, a numerical solution of OBEs is used in theoretical treatment of atomic system of two Λ schemes. In this work, interactions of four laser fields driving a double-Λ level scheme were analyzed using perturbative method to solve OBEs [7]. Perturbative method produces simpler solutions and analytical expressions can be obtained. The comparison of results obtained by using lower-order corrections of perturbative method and the exact calculations using optical Bloch equations will be presented. Analytical expressions provide valuable information on the mechanisms behind processes that occur in the double-Λ atomic system which cannot be deduced from numerical solutions of the OBEs for the same atomic scheme.

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Electronic densities associated with atomic resonances in laser fields

S. Vučić

Institute of physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

The study of the response of atoms embedded in strong laser fields provides the opportunity to study the matter-radiation interaction in the highly non-linear regime. Here, we consider hydrogen and argon atoms in a linearly polarized laser field of 800 nm wavelength with moderate to high intensity. The argon atoms may be well represented in strong fields by one valence electron moving in a resultant model potential [1]. The specific feature of an atom in an external field is that all the bound states decay after some finite lifetime. The energies of decaying "resonant" states are given by the positions of complex poles of the analytic continuation of the Green function beyond the real energy axes to the lower complex half-plane. The resonant lifetimes are related to the imaginary parts of the corresponding poles.

Here, we use the complex coordinate method [2] to solve spectral problem for the atom+field system without any approximation. The method known as "complex dilation" of the Hamiltonian enables direct access to positions and widths of the resonant states (and to associated wave vectors which are square integrable in the method). We represent the "active" atomic electron wavefunction by Floquet anzatz [3], which assumes the strict periodicity and the constant field amplitude during the interaction. We study the temporal dependence of the density of the probability represented in configuration space. Although the temporal dynamics of the wave function is not a physical quantity accessible to direct experimental measurement, it allows us to obtain important information about the internal processes in the atom.

For not too high field intensity and in non-resonant condition, the electronic densities of the ground- and low-excited states show small distortion along the polarization axes. When the field mixes the ground and an excited state, the electron oscillates with Rabi frequency between them. The radial distribution function shows complicated shape, corresponding to a linear superposition of the states. At sufficiently high intensities, the electron driven back and forth by the field, has a high probability of recolliding with the ionic core and be scattered in the polarization direction with a high velocity. Since the emission of low and high energy electrons are often completely dominated by series of multiphoton resonances, we study the temporal dependence of the electronic probability densities under various resonant conditions.

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Blackbody radiation induced excitation and decay of Rydberg states in potassium

I. L. Glukhov

Department of Physics, Voronezh State University, University square 1, 394006 Voronezh, Russia
E-mail: GlukhovOfficial@mail.ru

Photons of the ubiquitous blackbody radiation (BBR) perturb any quantum system unless it is placed in an environment at T = 0 K. Blackbody radiation causes ac-Stark shifts of states, a redistribution of population between states and ionization of neutral atoms. An account of BBR is especially important under investigation of Rydberg states at normal temperatures (T = 300 K) as the effect of BBR-induced transitions on such states is greater than the effect of spontaneous decays.

The rates of BBR-induced decay and excitation transitions from Rydberg states with principal quantum number *n* up to 100 in S-, P-, D-series of a neutral potassium were calculated in Fues' model potential (FMP) approach. It's interesting to note that the traditional FMP provides better agreement for rates of BBR-induced transitions with the [1] in S-series of potassium than the modified FMP [2].

The next two-step approximate formula is used as a compact representation of rates of BBR-induced decay $\left(P_{nl}^{dec}\right)$ and excitation $\left(P_{nl}^{exc}\right)$ for wide range of Rydberg states (with n up to 1000):

$$P_{nl}^{\mathrm{dec(exc)}} = \frac{a_0^{\mathrm{dec(exc)}}(1 + a_1^{\mathrm{dec(exc)}}x + a_2^{\mathrm{dec(exc)}}x^2 + a_3^{\mathrm{dec(exc)}}x^3)}{\exp[0.315775\Delta\mu x^3] - 1}, \quad x = \frac{100}{\nu T^{1/3}},$$

$$a_0^{\mathrm{dec(exc)}} = \mathrm{Const}, \quad a_i^{\mathrm{dec(exc)}} = b_{i0}^{\mathrm{dec(exc)}} + b_{i1}^{\mathrm{dec(exc)}}T^{-1/3} + b_{i2}^{\mathrm{dec(exc)}}T^{-2/3}, \quad i = 1, 2, 3.$$

The introduction of correction for quantum defect (Δμ) not only for S-series but also for P-and D-series improves a behavior of the approximation in the range of states corresponding the maximal rates at a given temperature (excitation rates according to approximation (solid lines) at both figures are compared with the results of direct FMP computations (crosses) for $P_{3/2}$-series).

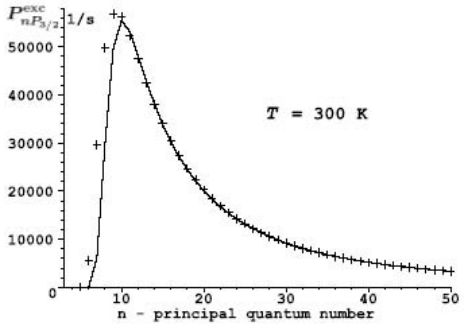

Fig.1. Approximation without the correction

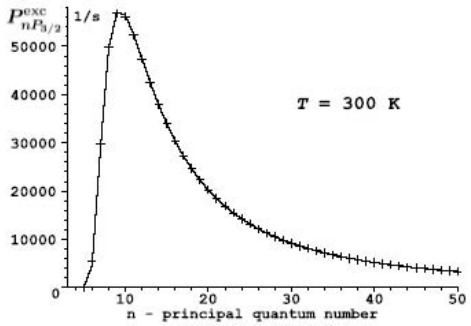

Fig.2. Approximation with the correction

Acknowledgments: Russian Foundation for Basic Research (grant No 11-02-00152-a), Dynasty foundation.

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Luminescence of exciplex XeCl*- and XeBr*- molecules excited by an electric discharge in the Xe/CsCl/CsBr gas-vapor mixture

M. Klenivskyi, V. Kelman, Yu. Zhmenyak and Yu. Shpenik

Institute of Electron Physics, National Academy of Sciences of Ukraine, 21, Universitetska Str., 88017 Uzhgorod, Ukraine

Investigations of emission spectral characteristics of an electric discharge in the triple mixture of Xe with CsCl and CsBr vapors were carried out in this research. Gas-vapor mixture was excited by longitudinal pulsed-periodic high-voltage electric discharge. Concentration of CsCl and CsBr molecules in the discharge volume was set by simultanious heating of CsCl and CsBr powders and was adjusted by corresponding temperature variation during the experiments. Saturated vapor pressure of CsCl and CsBr at 1 Torr is set at a temperature of about 1000 K.

Within the optimal excitation conditions the spectral composition of discharge radiation in the UV region was clearly characterized by the dominating intensity of the $B_{1/2} \rightarrow X_{1/2}$ band of exciplex XeCl* molecules and the less intense $B_{1/2} \rightarrow X_{1/2}$ band of exciplex XeBr* molecules with spectral maxima of radiation intensity at wavelengths 308 and 282 nm respectively. The structure of the discharge radiation spectra shows that mainly radiative transitions from the lowest vibrational levels of an electronic *B* state of exciplex molecules dominate in the emission.

Other two molecular bands which correspond to $D_{1/2} \rightarrow X_{1/2}$ radiative transitions of exciplex XeBr* (220 nm) and XeCl* (235 nm) molecules are noticeable in the discharge radiation spectra. In addition, cesium atom resonance line doublets in the IR, visible and UV spectral regions, namely the $6p \rightarrow 6s$ (852.1 + 894.3 nm), $7p \rightarrow 6s$ (455.5 + 459.3 nm), and $8p \rightarrow 6s$ (387.6 + 388.9 nm) transitions are present in the discharge spectra. The presence of cesium atoms in the discharge plasma is due to the chemical composition of the halogen carriers (CsBr and CsCl) and the main way of cesium atoms occurrence is associated with the production of the exciplex molecules.

The formation of exciplex molecules in this case takes place due to the substitution reactions which can occur simultaneously via two channels. In the first channel production of working molecules is realized by the substitution of alkali ion in the alkali halide molecule by rare gas ion (1), while in the second channel they are produced due to the substitution of alkali atom by rare gas in the excited state (2):

$$Rg^+ + AX \rightarrow RgX^* + A^+, \quad (1)$$

$$Rg^* + AX \rightarrow RgX^* + A, \quad (2)$$

where AX, RgX*, Rg, X, A are alkali halide molecule, exciplex molecule, rare gas, halogen atom and alkali metal respectively.

In both cases simultaneously with the formation of an exciplex molecule, cesium ion or atom as a by-product of substitution reactions are released, the resonance lines of which are observed in the spectral characteristics of the discharge radiation.

The results of the research have showed that working mediums on mixture of rare gas with alkali halide vapor can be alternative to traditional working mediums containing toxic halogen gas in manufacturing of exciplex sources of UV radiation. Besides the non-toxicity of halogen donor, investigated type of mixtures provides variation capacity of halogen carrier concentration in the already sealed bulb as well as long operating time of excilamp without replenishment of mixture components.

Time resolved laser induced fluorescence measurements: considerations when using Nd:YAG based system

M. S. Rabasović[a], D. Šević[a], M. Terzić[b], B. P. Marinković[a]

[a] *Institute of Physics, Belgrade, P.O. BOX 68, University of Belgrade, Serbia*
[b] *Faculty of Science, University of Novi Sad, Serbia*

Time-resolved laser-induced fluorescence (TR-LIF) and the laser induced breakdown spectroscopy (LIBS) have been shown to be methods which are fast and sensitive to provide information about the constituents in analyzed samples. TR-LIF and LIBS have similar hardware requirements. In this paper we analyze some characteristics of TR-LIF/LIBS system implemented in our laboratory [1], [2], [3], shown in Fig. 1, considering the fact that the excitation part of the system is based on Nd:YAG laser and Optical Parametric Oscillator (OPO). The laser is more than powerful enough (365 mJ at 1064 nm, variable OPO output >5mJ) for LIBS, but somehow slow (the length of fundamental laser harmonic output pulse is about 5 ns) for fluorescence measurements in our present area of interest, namely plants and food products. The pulse length of tunable OPO output (320-475 nm) could be reduced to shorter times, so by means of a correct deconvolution procedure it is possible to measure the fluorescence lifetimes in the range as small as a few nanoseconds. The fluorescence detection part of our system is based on picosecond streak camera. Using the fluorescent dyes (Rhodamine B and Fluorescein) ethanol solutions we verified the analyzing capabilities of our TR-LIF system.

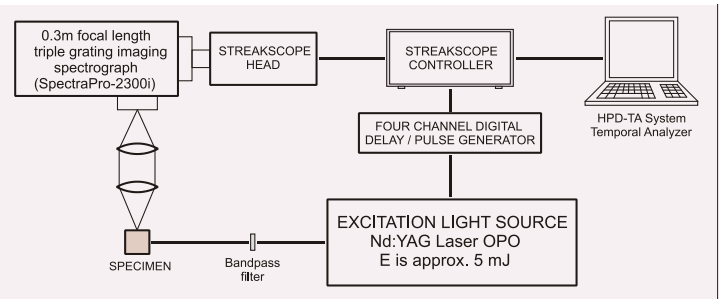

Fig. 1. Schematic illustration of experimental setup for TR-LIF spectroscopy

Acknowledgments: The work has been done within the project 171020 financed by the Ministry of Education and Science, Republic of Serbia and ESF COST Action FA0906 UV4growth.

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Detecting indium spectral lines using electron spectroscopy and laser induced breakdown spectroscopy

M. S. Rabasović[a], D. Šević[a], V. Pejčev[b], B. P. Marinković[a]

[a] *Institute of Physics, Belgrade, P.O. BOX 68, University of Belgrade, Serbia*
[b] *Faculty of Natural Science, University of Kragujevac, Serbia*

In this paper we present results regarding indium lines obtained by electron spectroscopy and laser induced breakdown spectroscopy. The resolution of our laser induced breakdown spectroscopy (LIBS) apparatus is better than when using electron spectroscopy. However, possibility of detection of optically forbidden transitions is an advantage of electron spectroscopy. The results that concern the elastic differential cross sections and resonant excitations of indium atoms are obtained using the electron spectroscopy in our laboratory and published recently [1,2]. An advantage of LIBS is the possibility of operation under normal temperature and air pressure. The optical diagnostics of indium lines could be useful for detecting indium in electric waste, because the detecting device could be made portable. Some preliminary results of detecting indium are presented in [3]. The most intense lines of the spectrum at 304 nm, 325 nm, 410 nm, 452 nm are detectible by both methods. Time resolved LIBS spectrum of pure indium is shown in Fig. 1.

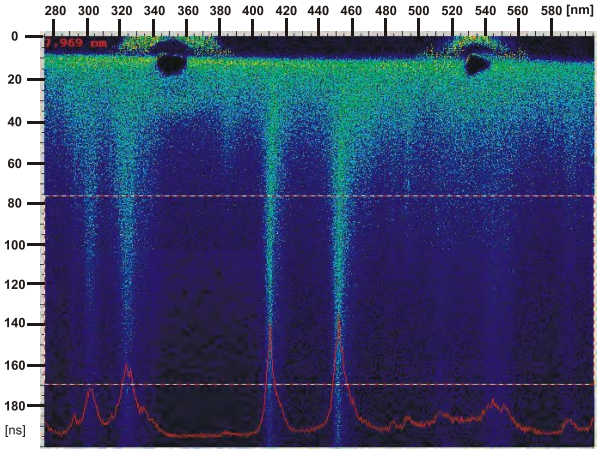

Fig. 1. Time resolved LIBS spectrum of indium.

Acknowledgments: The work has been done within the project 171020 financed by the Ministry of Education and Science, Republic of Serbia and ESF COST Action FA0906 UV4 growth.

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Nitrogen first negative system studied by electron induced fluorescence

J. Országh, M. Danko, M. Lacko, Š. Matejčík

Department of Experimental Physics, Comenius University, Mlynska dolina F-2, Bratislava, Slovakia, e-mail: orszagh@fmph.uniba.sk

Optical emission spectroscopy (OES) is an important toll to study the properties of the atmospheric pressure plasmas, or discharges. In the case of air the nitrogen molecule plays an important role in OES. The OES yields important information about the plasma and electric discharges, e.g., energy of the electrons, vibrational and rotational temperatures of the gas etc.

In this study the 1st negative system of nitrogen (N_2^+:$B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$) was examined by electron induced fluorescence method. The new crossed electron-molecular beam apparatus was used to study the nitrogen 1st negative system. The electron beam of approximately 90nA produced by trochoidal electron monochromator is colliding with molecular beam in the reaction chamber. The pressure of N_2 in the chamber is in the range of $1x10^{-4}$mbar. The photons produced in this region are collected by system of lenses and focused onto the entrance slit of an 0,75m optical monochromator. Then they are detected at the exit of monochromator by Hamamatsu R4220P photomultiplier. The spectrum with indentified transitions is shown in the figure 1.

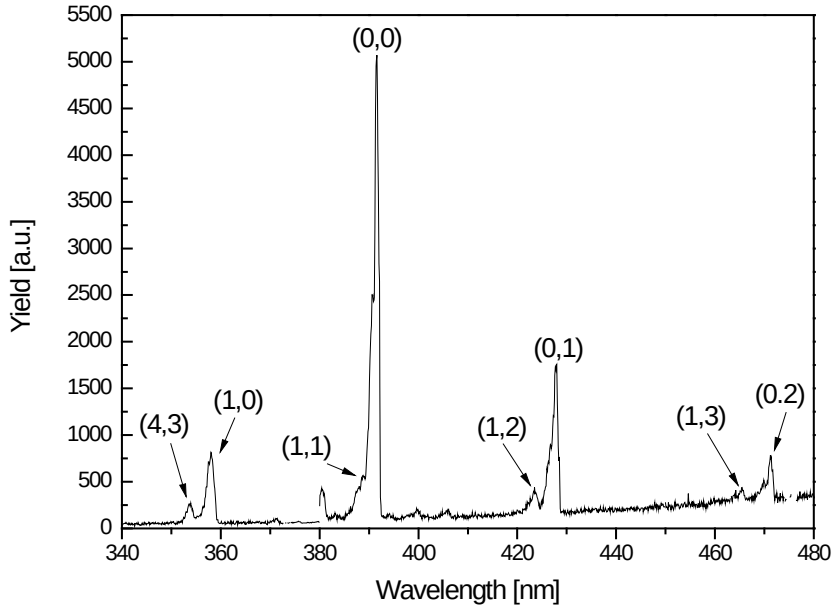

Fig.1. The EIF spectrum of nitrogen 1st negative system induced by electrons having kinetic energy of 50eV.

The relative cross-sections of several transitions were measured as well to find the threshold energy of these processes and the electron energy where the cross-section value reaches maximum.

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Optimizing the parameters for maximal ion extraction efficiency in Time-of-Flight mass spectroscopy

M. Popović[a] and G. Poparić[a]

[a]*Faculty of Physics, University of Belgrade, Studentski trg 12, 11000 Belgrade*

Low energy electron-molecule collisions are investigated by use of a crossed beam double trochoidal electron spectrometer and a Time-of-Flight mass spectrometry (TOF). Here we report some modifications in our former instrumentation [1], [2], now extended for measuring absolute DEA cross sections as well as for detecting small molecular ions. Slight changes are made by reducing the total number of electrodes in trochoidal electron spectrometer (particularly reducing the monochromator), and by adding a hole on one of two D-plates that form a collision chamber. The pulsing voltage is applied to the central U-plate opposed to the extraction hole, serving in this mode as repeller plate. Ions generated by electron scattering on molecules (through DEA mechanism) are
drawn out by repeller voltage and then analyzed using TOF technique [3]. We present optimum sequence of timing events in TOF, calculated for various repetition rates (from 10 to 20 kHz) and voltages applied to repeller.

Main task here is to collect and analyze the ions, as more as possible (in both total ion collection mode and TOF) by choosing the appropriate geometry of focusing elements system (electrostatic mirrors) and deflectors. Here we bring results of numerical simulations of ion trajectories under the various parameters of the system, performed in Simion 4.0. program. Following parameters were varied: external magnetic field (in range of 20 to 80 G), voltage on the target chamber walls, properties of the electrostatic mirrors (geometry, voltage), ion type (CH_3^+, OH^-, C_2H^-, H^-) and ion kinetic energy (0,1 to 5 eV) [4]. For this we calculated optimal conditions for maximal extraction efficiency, which is presented also as function of particular parameters. At the end, we compare our results with the literature data for similar system arrangements.

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Spin exchange asymmetry in the elastic electron scattering by Eu atom

V.I. Kelemen, E.Yu. Remeta

Institute of Electron Physics, 21 Universitetska str., 88017, Uzhgorod, Ukraine

The angular dependence of the spin exchange asymmetry $A=(\sigma^{\downarrow\uparrow}-\sigma^{\uparrow\uparrow})/(\sigma^{\downarrow\uparrow}+\sigma^{\uparrow\uparrow})$ was calculated in terms of the spin-polarized approach using the optical parameter-free potential $V_\lambda^\pm = V_s + V_e^\lambda + V_p^\lambda + V_{so}^\pm$ [1]. The differential elastic scattering cross sections $\sigma^{\downarrow\uparrow}$ and $\sigma^{\uparrow\uparrow}$ were calculated for the cases when the incident electron spin is antiparallel ($\lambda=\downarrow\uparrow$) and parallel ($\lambda=\uparrow\uparrow$) to the spin (7/2) of the Eu atom. The spin exchange potentials V_e^λ were taken in the free electron gas approximation. The polarization potentials V_p^λ have the incident electron spin-dependent short-range correlation part V_c^λ [1]. Two parts of the polarization potential, V_c^λ and the asymptotics $-\alpha_d/2r^4$, intersect at the $r_c^{\uparrow\uparrow}=9.544\,a_0$ and $r_c^{\downarrow\uparrow}=11.6\,a_0$ points. The dipole static polarizability α_d of the Eu atom is $204.4\ a_0^3$ [1]. The asymmetry is studied here using the potential $V2_\lambda^\pm$ as well, with the spin dependence being taken into account in V_e^λ only. The energies in fig. 1(a)-(c), at which the asymmetry almost reaches 100%, are the energies of the d- (at 1.3 eV) and f- (at 4.8 and 5.5 eV) shape resonances. The asymmetry value decreases with energy. In the vicinity of the critical minimum [36.8 eV, 141.6°] (see fig. 1(d)) it reaches the larger values showing a drastic behavior. The calculation using the potential $V2_\lambda^\pm$ at 4.8 eV provided the asymmetry sign change at 130°.

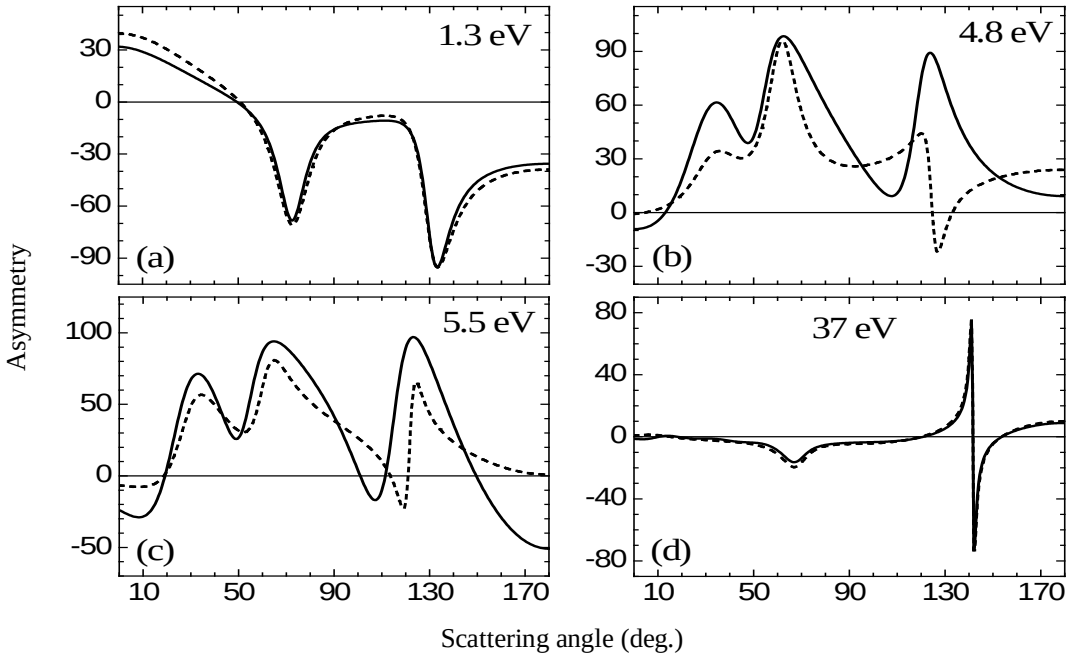

Fig. 1. Angular dependence of the spin exchange asymmetry $A(E,\theta)$ (in %) for the elastic electron scattering by the Eu atom. The results are obtained using the $V_\lambda^\pm$ (solid line) and $V2_\lambda^\pm$ (dashed line) potentials.

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Experimental (e,2e) study of resonant Auger states of Ar

B. Paripás[a], B. Palásthy[a] and M. Žitnik[b]

[a]*Department of Physics, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary*
[b]*J. Stefan Institute, Jamova 39, P.O.B. 3000, SI 1000, Ljubljana, Slovenia*

Electron spectra emitted after 2p inner-shell excitation of argon were studied by (e,2e) coincidence technique based on cylindrical mirror analyzers [1]. The transmitted energy to the atom – i.e. the energy difference of the primary and scattered electrons - corresponded to the energy positions of Ar L_3 inner-shell excited atomic states. Particularly the 2p→4s (244,4 eV) and the dipole forbidden 2p→4p (245,7 eV) excitations were studied extensively. The resonant Auger spectra were obtained by the removal of the background caused by the outer-shell electrons. The latter was measured at about 240 eV transmitted energy, where the inner-shell processes are not possible.

The spectra reported by our group represent the first experimental data concerning resonant Auger spectra emitted upon electron impact excitation [2,3]. In particular, the resonant Ar[$2p_{3/2}$]4p Auger spectrum is reported for the first time. The 4s spectrum displays a substantially larger shake-up contribution than the one observed in photoexcitation experiments, which may be explained by the interference of the resonant decay path with the direct ionization-excitation of the Ar 3p subshell.

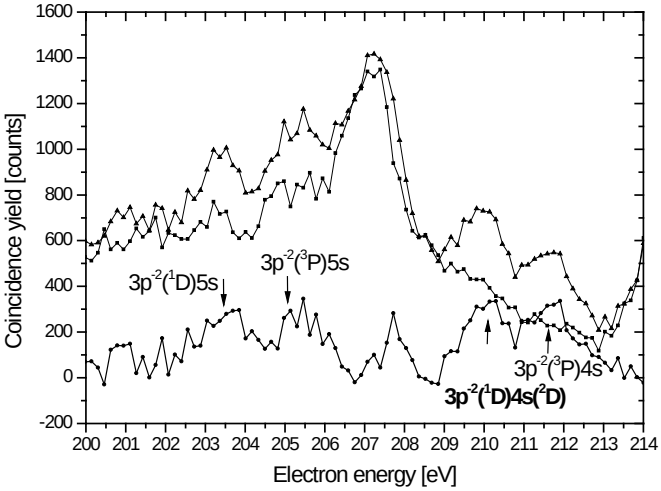

Fig.1. The resonant Auger spectrum emitted by Ar[$2p_{3/2}$]4s state (thick line with circles), obtained as a difference of (e,2e) spectrum measured at E_0 =343.6 eV (thin lines with triangles) and the direct ionization background (thin lines with squares).

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K-shell ionization of Cu by positron impact

T. Mukoyama[a], Y. Nagashima[b], and K. Tőkési[a]

[a]*Replace this text with authors' affiliations [1]Institute o f Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary*
[b]*Department of Physics, Tokyo University of Science, 1-3, Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan*

In recent years several experimental efforts have been made to measure absolute K-shell ionization cross sections of copper by positron impact [1]. The measurement was based on the accurate observation of the characteristic x-rays following the inner-shell ionization.

In this work K-shell ionization cross sections of copper are studied theoretically. We applied the binary encounter approximation (BEA) and a classical trajectory Monte Carlo (CTMC) method. In both cases we used the frozen charge state model and we used the Slater-rule for the determination of the static nuclear charge of 1s electron bound to the copper nucleus. The present calculations were performed solving the non-relativistic equations.

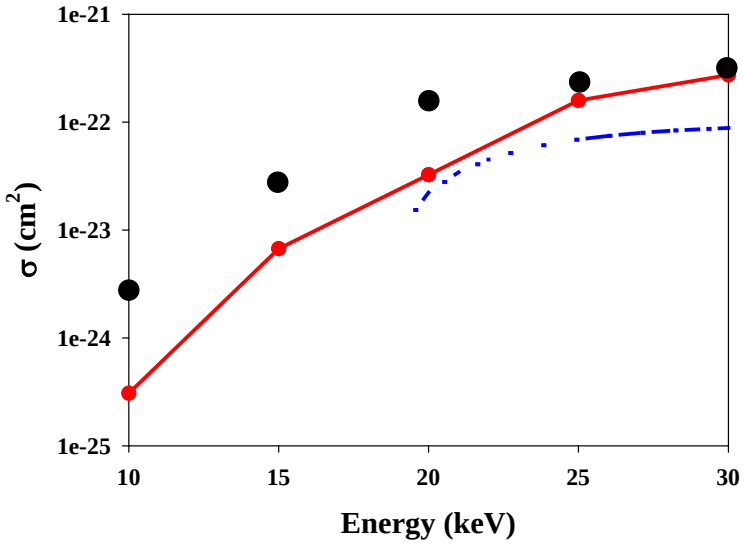

Fig.1. K-shell ionization cross sections of Cu by positron impact. Solid circle: Experimental data from ref. [1], solid line: present CTMC data, dashed line: binary encounter approach.

Fig. 1 shows the K-shell ionization cross sections of Cu as a function of the positron impact from the threshold energy up to 30 keV. While the CTMC data are relatively close to the experimental data the BEA data underestimate those ones. We note, however, that applying the relativistic velocity distribution for atomic electrons, the BEA values are increased and thereby ensured better agreement with the measured values.

Acknowledgments: This work was supported by the Hungarian Scientific Research Fund OTKA No. K72172.

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State selective electron capture in low energy positron and argon collisions

K. Tőkési

Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary

High-resolution measurements of positronium formation total cross sections in positron and argon atom collisions are recently available [1]. The measurements were performed at low energy positron impact, from the threshold energy up to 60 eV.

In this work the positron and argon atom collisions is studied theoretically. We treat the collision problem in the framework of a classical trajectory Monte Carlo (CTMC) model. The CTMC method is a nonperturbativ method, where classical equations of motions are solved numerically. In the present work the CTMC simulations were made in the three-body approximation i.e. the many-electron target atom was replaced by a one-electron atom. The argon ion (including the other electrons) is represented by a model potential. The detail of the calculation procedure is found in ref [2].

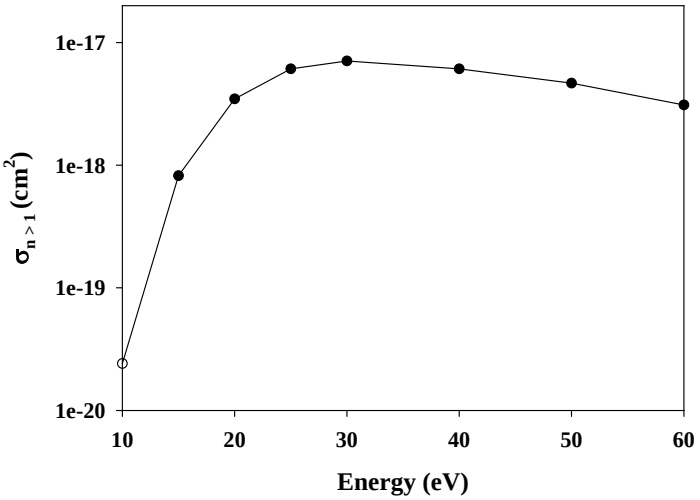

Fig.1. Total capture cross sections from Ar(3p) into the excited states of the positron as a function of positron impact energies.

Beside the total cross section data, we present state selective (n,l) positronium formation cross sections in collision between positron and argon atom as a function of the incident projectile energy. Fig. 1 shows the total capture cross sections from Ar(3p) into the excited states of the positron (n>1) as a function of positron impact energies.

Acknowledgments: This work was supported by the Hungarian Scientific Research Fund OTKA No. K72172.

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Possible structure of electron and positron

N. V. Delić, J. P. Šetrajčić, S. Armaković, I. J. Šetrajčić

Faculty of Sciences, Department of Physics, University of Novi Sad, Serbia

The hypothesis is that the photon [1] is a bound state of neutrino and antineutrino. This hypothesis has been sent to CEWQO Symposium 2010 [2]. The hypothesis that the photon bound states of the neutrino and antineutrino has resulted in the first place that there are three types of photons, due to the fact that there are three types of neutrinos: electron, muon and tau neutrino. Since there are three types of interaction of photons with matter, namely: photoelectric effect, Compton effect and electron positron pair production, we shall see how it functions within our theory of the photon as a bound state of the neutrino and antineutrino. Here it is necessary to introduce one more assumption about the electron bound states. From the standpoint of current science known facts about W minus bosons is "W-bosons decay to produce either a quark and a differently charged antiquark or a charged lepton and a neutrino (or antineutrino)." This conclusion should be replaced with the hypothesis that the electron is bound states of W minus bosons and neutrinos [3].

$$e^- = (W^- + \nu_e) = W^- \nu_e, \quad e^+ = (W^+ + \overline{\nu}_e) = W^+ \overline{\nu}_e \tag{1}$$

The fact that the electron mass is around 160 000 times smaller than the associated weight W minus boson has so far resulted in the negative W boson decays into an electron and electron antineutrino. From the perspective of our interpretation, of minus W boson, cannot exist independently, in order to survive is linked electron neutrino from photon in cosmic ray (other particle is electron antineutrino is detect) and provides a stable electron structure of the material. Come up with Wave-energy-information transformation into a stable material (it must be made to work to form a stable substance, and this requires energy) in our view that the energy conservation law is valid. From the perspective of our interpretation, the graviton is a hypothetical elementary particle responsible for equations (1) that mediates the force of gravitation in the framework of quantum field theory.

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The collinear versus 3D adiabatic model for helium atom in hyperspherical coordinates

N. Simonović

Institute of Physics, University of Belgrade, P.O. Box 57, 11001 Belgrade, Serbia

The collinear models of helium atom, where the electrons reside on the opposite sides of the nucleus (eZe configuration) and on the same side (Zee configuration), are studied using the adiabatic approach in hyperspherical coordinates [1,2]. The adiabatic potential curves and energy levels (within the single-channel approximation) for the collinear atom are compared to those for the full 3D model (Fig. 1). It is shown that the S states of the 3D model with minimal and maximal angular excitations, as well as the corresponding adiabatic potential curves at large values of the hyperradius, can be related to the eZe and Zee collinear configurations, respectively. It is demonstrated that a set of curves of the 3D atom converging to the same ionization threshold is confined in the area delimited by the pair of eZe/Zee curves also converging to this threshold. A class of anticrossings of the adiabatic potential curves in the 3D model, located along the eZe adiabatic curves at small values of the hyperradius, is observed and related to the unstable character of the classical configuration corresponding to the eZe collinear model in this domain [2].

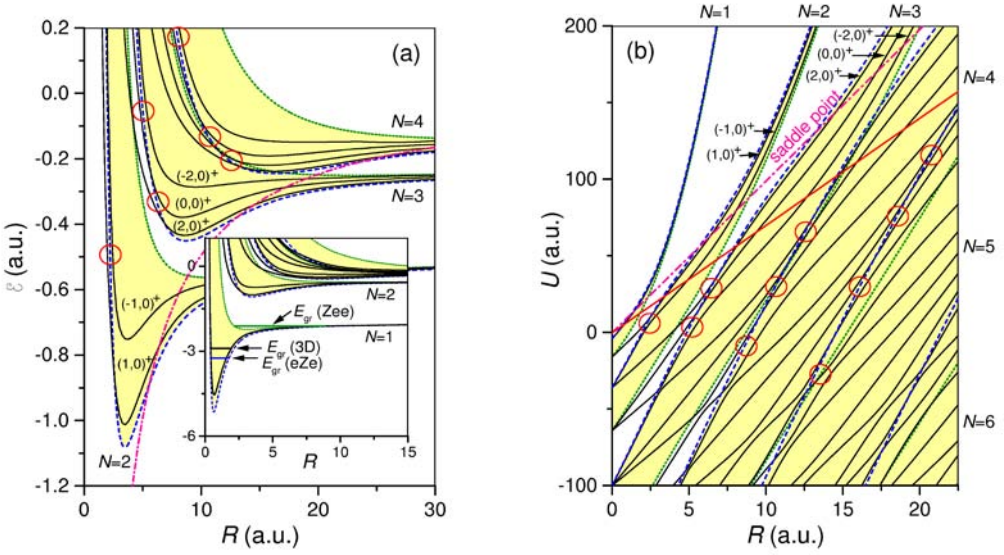

Fig. 1. $^1S^e$ hyperspherical curves for the full 3D helium atom (full black lines): (a) adiabatic energies ϵ and (b) adiabatic potentials U, and the areas (yellow) bounded by the corresponding curves for the eZe and Zee configurations of the collinear atom (dashed blue and dotted green lines). The ground state energies for the collinear configurations and for the 3D case are shown in the inset in part (a). The saddle point energy $E_{sp}(R)$ and the related function $U_{sp}(R)$ are drown by dash-dot pink lines. The red circles denote anticrossings of the 3D adiabatic curves, whereas the full red line (in part (b)) separates the areas with and without anticrossings.

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Altitude distribution of electron concentration in the ionospheric D-region in presence of time-varying solar radiation flux

A. Nina[a], V. Čadež[b], D. Šulić[c], V. Srećković[a]

[a]*Institute of Physics, University of Belgrade, P.O. Box 57, 11001Belgrade, Serbia*
[b]*AstronomicalObservatory, Volgina 7, 11060 Belgrade, Serbia*
[c]*Faculty of Ecology and Environmental Protection, Cara Dušana 62, 11000 Belgrade, Serbia*

Electron concentration distribution in the ionospheric D-region is very important for transmission of radio signals. Structure and characteristics of the sunlit ionosphere is not constant, it varies depending on solar activity (such as flares) which has been analyzed in many papers ([1], [2]).

During solar flares, the resulting radiation is increased and, consequently, the rate of photo-ionization processes and electron concentration is raised. In the after-flare phase when the radiation flux decreases in time, recombination processes (electron-ion, ion-ion and three body recombination) are dominant and electron concentration decreases and approaches values of the unperturbed ionosphere. Time periods of increasing and decreasing electron concentration can be named photo-ionization and recombination regime, respectively.

In this work, we study the influence of X ray solar flare recorded by GOES-15 satellite in March 24, 2011 from 12:01 to 12:11 UT. Time and altitude dependent characteristics of the ionosphere are calculated by using the amplitude and phase variations of VLF signals emitted by the DHO/23.4 kHz transmitter (Germany) that were registered in Belgrade by the AWESOME receiver system and numerically processed by the LWPC computing program [3]. In Fig. 1, time variations of electron concentrations are shown for three different altitudes together with time distribution of the solar flux.

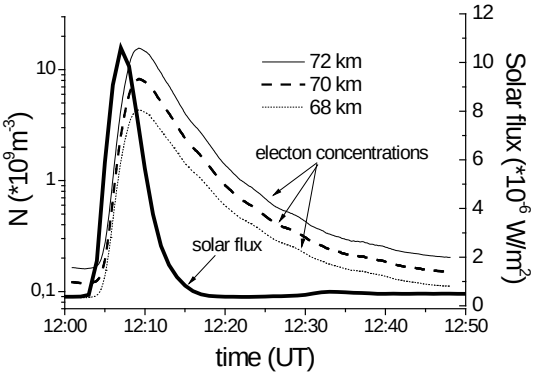

Fig.1. Obtained time evolutions of electron concentrations in the photo-ionization and recombination regimes at given altitudes, and solar flux recorded by GOES-15 satellite.

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Effective electron recombination coefficient in the ionospheric D-region during the relaxation regime following a solar flare on February 18, 2011

A. Nina[a], V. Čadež[b], D. Šulić[c], V. Srećković[a], V. Žigman[d]

[a]*Institute of Physics, University of Belgrade, P.O. Box 57, 11001Belgrade, Serbia*
[b]*AstronomicalObservatory, Volgina 7, 11060 Belgrade, Serbia*
[c]*Faculty of Ecology and Environmental Protection, Cara Dušana 62, 11000 Belgrade, Serbia*
[d]*University of Nova Gorica,Vipavska 13,Rožna Dolina, SI-5000 Nova Gorica, Slovenia*

During solar flares, the electron concentration is raised due to increased photo-ionization. At heights around 70 km, the dominant relaxation processes are the electron-ion, ion-ion and three-body recombination. These electron loss processes are characterized by a common effective recombination coefficient α [1].

In this paper, we calculate the time dependence of effective recombination coefficient α for different altitudes in the after-flare regime. The considered class M1.0 X-ray solar flare was recorded by GOES-15 satellite on February 18, 2011 between 14:00 and 14:15 UT. Our analyses use data on ionospheric electron distribution profiles computed from amplitude and phase variations of VLF signal emitted by the DHO/23.4 kHz transmitter in Germany and registered by the Belgrade AWESOME receiver system.

Fig. 1 shows the computed time distribution of the recombination coefficient α. The obtained values range within interval 10^{-12} – 10^{-11} m^3/s which is in agreement with values derived from analyses of other events such as red sprites [2], auroral electron precipitation [3], etc.

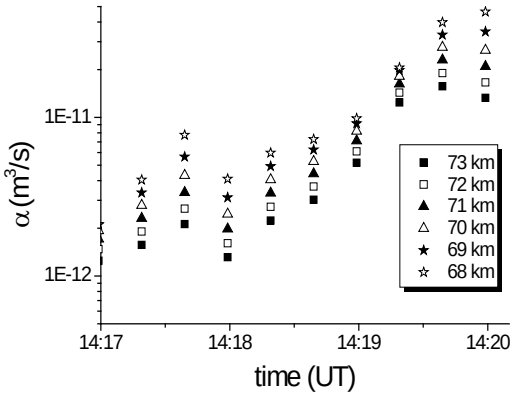

Fig.1. Time distribution of the effective recombination coefficient in after-flare regime at different altitudes

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Title of the Monte Carlo modeling of electrons and heavy particles in pure H_2 discharge

V. Stojanović, Ž. Nikitović and Z. Lj. Petrović

Institute of Physics, Pregrevica 118, 11080 Belgrade, Serbia

In this paper we show results of Monte Carlo modeling of electrons and heavy particles induced spatially resolved emission intensity and the Doppler profile of Hα line in pure H_2 discharge focusing on anisotropy of elastic scattering of heavy particles. For most intense inelastic scattering processes of heavy particles we used simplest assumptions. In particular we present study where transport of H^+ and fast H particles is modeled by anisotropic scattering. For H^+, H_2^+, H_3^+, fast H and H_2 we modeled scattering at the surface and of the molecules. Electron transport is also modeled by using available differential scattering cross sections. Anode and cathode boundaries are taken into account regarding electrons and heavy particles [4]. In order to achieve consistency with results of other authors we select conditions of simulation appropriate for moderate E/N (E-electric field, N-gas density) that are selected from experimental Townsend discharges in pure H_2.

In this study we used cross sections sets of Phelps [1] for H_3^+ ions transport, while for other particles we used data in [2]. For H^+ ions transport in this study we used either momentum transfer cross section of Phelps [2] or total cross section of Krstić and Shultz [3] for elastic scattering with differential cross section and for first three vibrational channels [3] of excitation asuming forward scattering. Surface effects to heavy particle transport are accounted for by using reflection coefficients for heavy particles from [2] and cosine angular distribution of reflected fast H.

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Numerical modeling of positronium thermalization

S. Marjanović [a], M. Šuvakov [a], J. J. Engbrecht [b], Z. LJ. Petrović [a]

[a] *Institute of physics, Belgrade, Pregrevica 118, 11080 Zemun*
[b] *Saint Olaf College, Northfield, Minnesota 55057, USA*

We will presented a numerical study of Positronium (Ps) thermalization in pure helium (He). Recent measurements of Ps thermalization yielded data that were analyzed to produce the scattering cross sections in helium [1] by using energy Balance equations with an assumption of Maxwell Boltzmann distribution (MBD) function for Ps. We have applied a Monte Carlo code to test the cross sections. As our code was developed without any approximations for the energy distribution function we have effectively also tested the assumptions and the validity of the simple theory used in [2]. We will present the simulation results in the form of thermalization profiles for several theoretical and measured cross sections. Also, the temporal evolution of energy distributions will be shown along with diffusion coefficients and spatial ranges of penetration. The thermalization of the initial distribution is rapid and the data follow relatively closely, those calculated in [1]. In principle this supports the choice of MBD and the cross section found in [1]. However the distribution function most of the time deviates from the MBD due to strong scattering. Finally, we applied the same procedure to analyze Ps thermalization in water vapour.

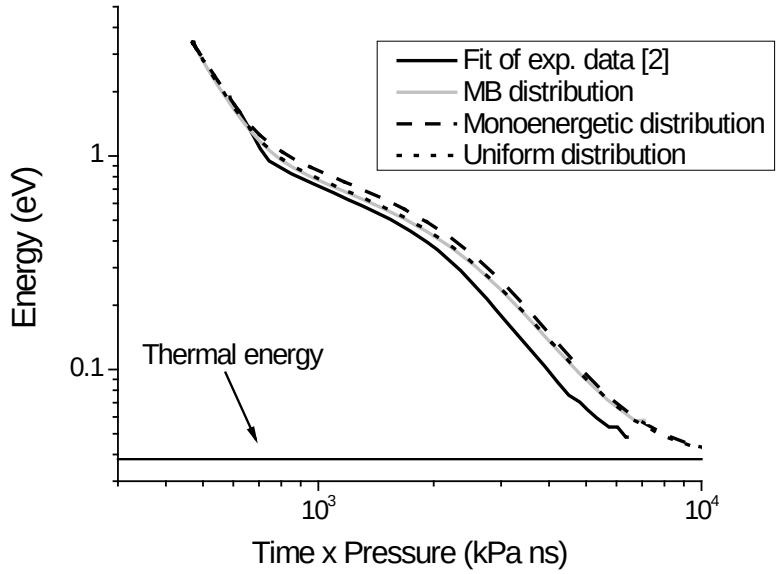

Fig.1. Comparison of thermalization profiles for different starting energy distributions.

Acknowledgments: Institute of Physics Belgrade, Serbian Academy of Sciences and Arts, Ministry of Science and Technological Development of Republic of Serbia.

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Modelling of microhollow cathode dsicharges in argon at atmospheric pressures

M. Radmilović-Radjenović, B. Radjenović, M. Savić

Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Studies of microhollow cathode discharges (MHCD's) are of interest, not only for the plasma community, but also for a number of applications based on their unique characteristics such as presence of intense excimer radiation and significant gas heating within the submillimeter discharge volume. As complement to the various experimental techniques, for studies of MHDC's different simulation techniques have been developed. This paper contains results of modelling of MHCD's in argon at atmospheric pressure achieved by using a two-dimensional Particle-in-cell code (XOOPIC) [1]. Simulation conditions were based on the experimental set-up and conditions described in ref. [2]: 100 μm thick electrodes separated by a 250 μm dielectric with opening of 200 μm. The gas pressure was varied between 12 and 500 Torr.

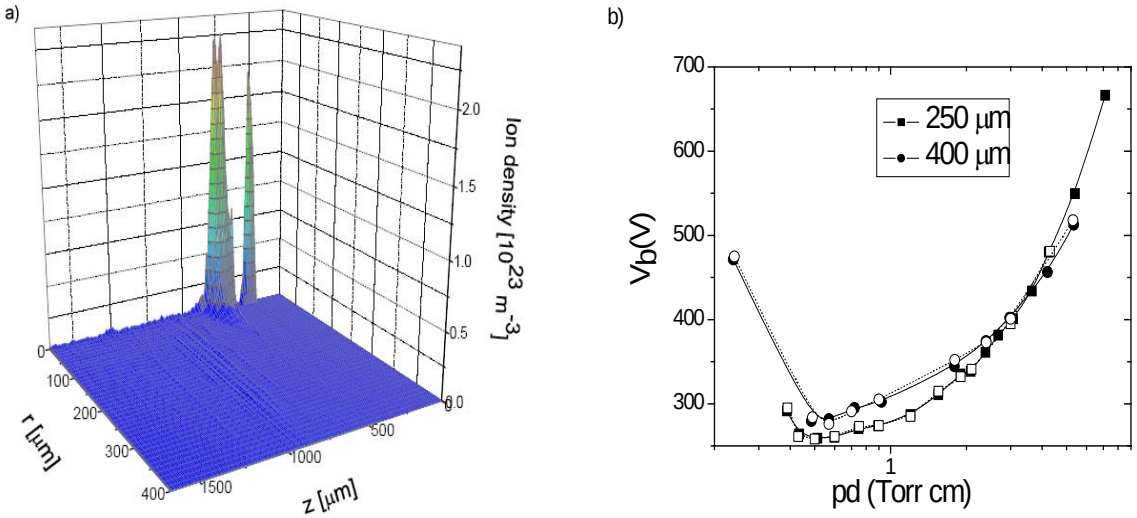

Fig.1. a) Density of ions in MHCD operated in argon at the pressure of 40 Torr and b) breakdown voltage curves for MHCD in argon for two different gaps. The experimental data from [2] are represented by solid dsymbols while open symbols coorespond to the simulation results.

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The secondary emission coefficient for air

M. Klas[a] , Š. Matejčik[a], B. Radjenović [b], M. Radmilović-Radjenović[b]

[a]*Department of experimental Physics, Comenius University, Mlynská dolina F2, 84248*
[b]*Institute of Physics,University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

The air is the cheapest and most widely used gase for circuit breaking since it can be compressed to extremely high pressures at room temperature. This paper contains experimental and simulation results for the DC breakdown voltage curve in dry air Based on the analysis of the the experimentally recorded breakdown voltage curve, the secondary emission coefficient γ as a function of the reduced electric field E/p has been estimated. In addition, Particle-in-cell/Monte Carlo collision (PIC/MCC) simulations have been performed [1,2]. A good agreement between experimental and simulation results can be found. The results, presented here, should be useful for determining minimum ignition voltages in microplasma sources as well as the maximum safe operating voltage and critical dimensions in other microdevices.

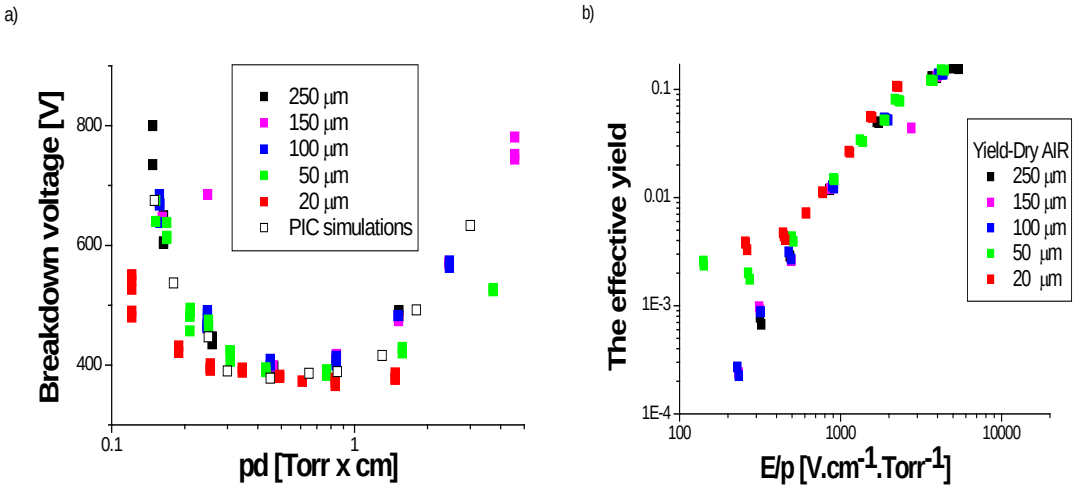

Fig.1. Comparison between experimental results (solid symbols) and PIC/MCC simulation results (open symbols) for: a) the breakdown voltage curve and b) the effective yield versus the ratio E/p in dry air.

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Monte Carlo simulation and Boltzmann equation analysis of non-conservative positron transport in H_2

A. Banković[a], S. Dujko[a,b], R. D. White[b], S. J. Buckman[c], Z. Lj. Petrović[a]

[a]*Institute of Physics, Pregrevica 118, 11080 Belgrade, Serbia*
[b]*ARC Centre for Antimatter-Matter Studies, James Cook University, Townsville 4810, Australia*
[c]*ARC Centre for Antimatter-Matter Studies, Australian National University, Canberra, ACT 0200, Australia*

This work reports on a new series of calculations of positron transport properties in molecular hydrogen under the influence of spatially homogeneous electric field. Calculations are performed using a Monte Carlo simulation technique [1,2] and multi term theory for solving the Boltzmann equation [3]. Values and general trends of the mean energy, drift velocity and diffusion coefficients as a function of the reduced electric field E/N are reported here. Emphasis is placed on the explicit and implicit effects of positronium (Ps) formation on the drift velocity and diffusion coefficients. Two important phenomena arise; first, for certain regions of E/N the bulk and flux components of the drift velocity and longitudinal diffusion coefficient are markedly different, both qualitatively and quantitatively. Second, and contrary to previous experience in electron swarm physics, there is negative differential conductivity (NDC) effect in the bulk drift velocity component with no indication of any NDC for the flux component. In order to understand atypical manifestation of the drift and diffusion of positrons in H_2 under the influence of electric field, the spatially dependent positron transport properties such as number of positrons, average energy and velocity and spatially resolved rate for Ps formation are calculated using a Monte Carlo simulation technique. The spatial variation of the positron average energy and extreme skewing of the spatial profile of positron swarm are shown to play a central role in consideration of the phenomena.

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Transport properties of positive ions in BF_3 plasmas

V. Stojanović[a], Z. Raspopović[a], J. Jovanović[b], S. Radovanov[c], Ž. Nikitović[a] and Z. Lj. Petrović[a]

[a]*Institute of Physics, University of Belgrade, Pregrevica 118, PO Box 68, 11000 Belgrade, Serbia*
[b]*Faculty of Mechanical Engineering, University of Belgrade, 11000 Belgrade, Serbia*
[c]*Varian Semiconductor Equipment Associates, 35 Dory Road, Gloucester, Massachusetts 01930*

This is Boron produced in plasma devices continues to be the main p-type dopant in ion implantation of semiconductor devices. Yet plasma parameters of most frequently used boron rich gases (BF_3, B_2F_6, $B_{10}H_{14}$) that determine the plasma content and beam quality are still not known.

Time resolved measurements of ion energy distributions in cathode boundary [1] of a pulsed dc plasma doping system revealed possible role of charge-transfer collisions between single charged ions of various mass.

The cross sections for scattering of B^+, BF^+ and BF_2^+ ions on BF_3 molecule are calculated by using Nanbu's theory [2,3] separating elastic from reactive collisions.

Monte Carlo simulation was applied to perform calculations of transport parameters as well as rate coefficients in DC electric fields. In Figure 1 we show mean energy as a function of reduced electric field E/N (E-electric field, N-gas density) for B^+, BF^+ and BF_2^+ ions in BF_3 gas.

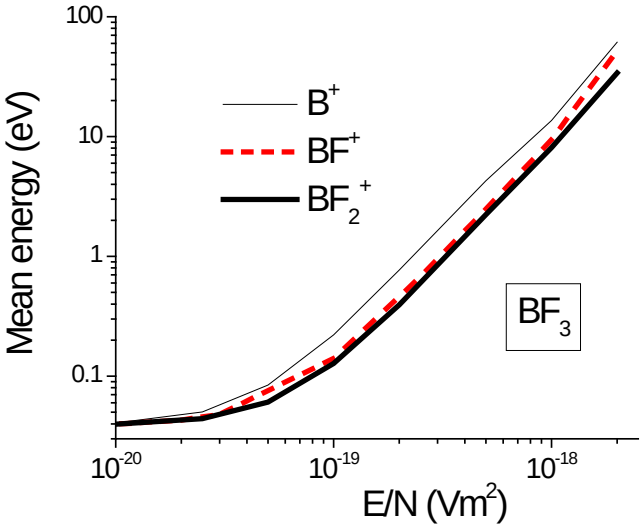

Fig.1. Mean energy of boron containing ions in BF_3 gas

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Contribution of near threshold states to dielectronic recombination in Li-like Al and C ions

V. Stancalie

National Institute for Laser, Plasma and Radiation Physics, Department of Lasers, P.O.Box MG-36, Magurele, 077125 ROMANIA, Association EURATOM/MEdC

Dielectronic recombination (DR) is the dominant electron-ion recombination process in both photoionized and electron-collisional plasmas. The basic process of interest is:

$$e^- + X^{Z+}(1s^2 2s(^2S^e)) \Leftrightarrow X^{(Z-1)+**}(1s^2\, 2p\, n'\, l') \rightarrow X^{(Z-1)+*}(1s^2 2s\, n'l') + h\nu \quad (1)$$

The incident electron is captured by the Li-like ion into a doubly excited resonant state, which can decay, either by electron emission or by photon emission. In the latter case the resultant ion state can be a bound state, and hence we have recombination. In the above equation X^{Z+} signifies the Li-like ion, of nuclear charge Z, in its ground state, and $X^{(Z-1)+**}$ is the doubly excited state of the corresponding Be-like ion of nuclear charge (Z-1). This state can decay by radiative transition to other excited state $X^{(Z-1)+*}$. If the resonance is at positive energy, the rate coefficient is commonly calculated in the 'isolated resonance' approach. In a simple picture, the strength of this positive energy resonance (integrated cross section) is proportional to the ratios $\Gamma_R\, \Gamma_A/ (\Gamma_R + \Gamma_A)$, where Γ_R and Γ_A are the radiative and autoionization transition probabilities, respectively.

Recently [1, 2], it has been pointed out the role of including negative energy resonant states into the general programs of DR for plasma modeling. The contribution of this 'compact class' of doubly excited states, moved down below threshold, depends on the resonance energy, E_R , and might be greater comparing with the contribution from positive energy resonance states which does not depend on whether E_R is positive or negative. This idea represents a novel challenge for atomic experiments, where the only positive energy resonances have been considered up to now.

If the resonance is at negative energy, the probability to be in an *n* manifold with total angular momentum J_r and core electron(s) with angular momentum J_c is given by[1]:

$$P(n, J_r) = \left(\frac{2\pi}{3}\right)^{3/2} \frac{2J_r + 1}{2(2J_c + 1)} \exp(-E_n / T)\zeta(E_n) \quad (2)$$

where $E_n = -Z^2/(2n^2)$ is the energy of the *n* manifold and $\zeta(E_n)$ is the Saha-Boltzman deviation factor.

In the present work it is suggested that the R-matrix Floquet (RMF) theory and code, and its extension to Laser Induced Degenerate State phenomenon (LIDS) [3,4 and references herein], should be used to treat DR process, accounting for the positive and negative energy resonances contribution, in a consistent way. We present comparative results, from the RMF and the low-order relativistic calculation, using a multi-configuration Dirac-Fock (DARC) atomic structure code, for radiative and autoionization rates. Application refers to Li-like Al and C ions.

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Elastic electron scattering from formamide molecule

J. B. Maljković[a], F. Blanco[b], G. García[c], B. P. Marinković[a] and A. R. Milosavljević[a]

[a]*Laboratory for Atomic Collision Processes, Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[b]*Departamento de Física Atómica Molecular y Nuclear, Facultad de Ciencias Físicas, Universidad Complutense, Avda. Complutense s/n, E-28040 Madrid, Spain*
[c]*Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 121, 28006 Madrid, Spain*

In the present contribution, both experimental and theoretical results on elastic electron interaction with formamide molecule are reported. Measurements were performed using a cross beam technique [1], for scattering angles from 20° to 110° and for the incident energies from 50 to 300 eV. The calculations of molecular cross sections are based on a corrected form of the independent-atom method, known as the SCAR (Screen Corrected Additivity Rule) procedure [2]. Regarding the shape of differential cross sections, experimental and theoretical results agree well.

The formamide molecule represents the smallest system containing the peptide bond. Therefore, the investigation on electron interaction with formamide can be useful to understand processes of low-energy electron-protein interactions, as well as for interstellar research [3].

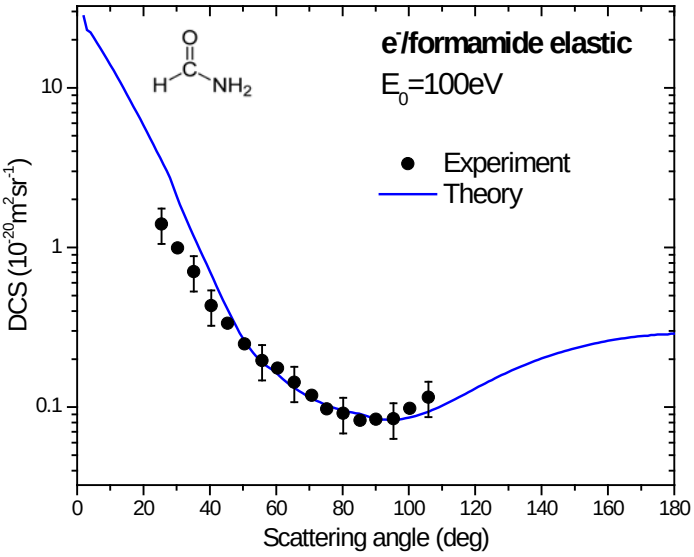

Fig.1. Angular dependence of relative DCSs for elastic electron scattering from formamide molecule at electron energy of 100eV: (—), theory; (●), experiment (normalized to the theory).

Acknowledgments: The work was supported by the Ministry of Education and Science of Republic of Serbia (Project No. 171020) and Spanish Ministerio de Ciencia e Innovación Project FIS2009-10245, and motivated by COST projects ECCL and Nano-IBCT.

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Electron impact ionization and electron attachment to Gly-Gly in a gas phase

M. Stano, P. Papp, K. Pisklová, Š. Matejčík, J. Urban

Faculty of mathematics, Physics, and Informatics, Comenius University, Mlynska dolina, 842 48 Bratislava, Slovakia

Low energy electrons which are produced in vast amount by absorption of a high-energy radiation in matter have been recognized to play a key role in radiation damage of biological systems. It has also been shown that low energy electrons can seriously damage biological molecules and polymers [1]. Study of electron interactions with small peptide molecules is therefore important for better understanding of the processes involved [2].

Here we present an experimental study of electron induced reactions in a gas phase Gly-Gly. The work is done on a crossed electron/molecular beam apparatus consisting of a heated effusive molecular beam source, trochoidal electron monochromator and a quadrupole mass spectrometer.

Formation of negative ions is observed at two resonancies close to 0 eV and at about 1 eV. Negative ions with mass 131, 113 and 46 amu have been observed. Electron impact ionization of Gly-Gly has been studied at low energies close to ionization thresholds. Appearance energies of parent and fragment ion formation have been evaluated using a fitting procedure involving a convolution of electron energy distribution function and expected cross section dependence.

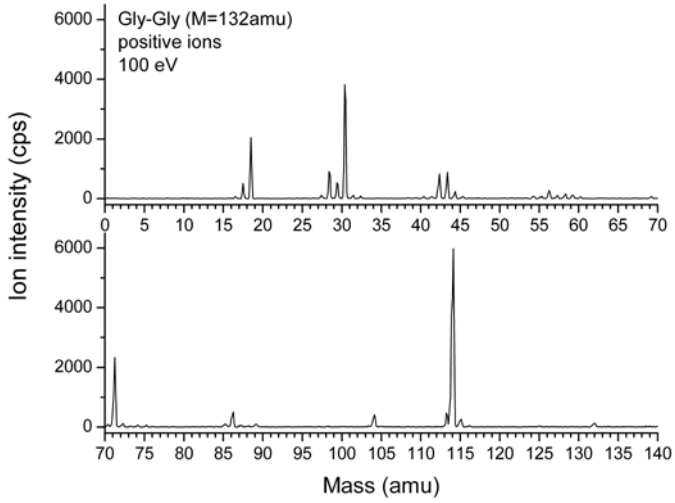

Fig.1. Mass spectrum of positive ions formed by electron impact ionization of Gly-Gly at 100 eV.

Acknowledgments: This work was supported by the Slovak Research and Development Agency grant APVV 0310-07, SK-SRB-0011-09 and by slovak grant agency VEGA, project VEGA-1/0558/09.

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Combined experimental and theoretical study of electron impact ionization of $Co(CO)_3NO$ molecule

P. Papp[a], M. Stano[a], S. Engmann[b], P. Mach[c], O. Ingolfsson[b], Š. Matejčík[a]

[a]*Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Mlynská dolina, 842 48 Bratislava, Slovakia*
[b]*Science Institute, University of Iceland, Dunhaga 3, 107 Reykjavik, Iceland*
[c]*Department of Nuclear Physics and Biophysics, Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Mlynská dolina, 842 48 Bratislava, Slovakia*

This work is focused on electron impact ionization (EII) and related dissociations studies of organometallic compound cobalt tricarbonyl nitrosil ($Co(CO_3)NO$), which belongs to the group of widely used compounds in plasma technology and nanotechnologies as precursors for preparation of thin metallic layers. The crossed electron molecular beams technique [1] was used to measure the mass spectrum of positive ions formed by EII and the appearance energies of fragmented ions. Moreover, bond dissociation energies have been evaluated from the experiment.

According to our previous experiences with theoretical modeling of fragmentation reactions using the recent methods of quantum chemistry we have performed several calculations in GAUSSIAN 03 program package [2]. The Density Functional Theory methods have been selected [3] for obtaining the optimal geometries of parent molecule [4], its positive ion and of each fragmented product, positively charged and neutral. From the DFT energies of fragments the reaction energies and bond dissociation energies were calculated and compared to the experiment.

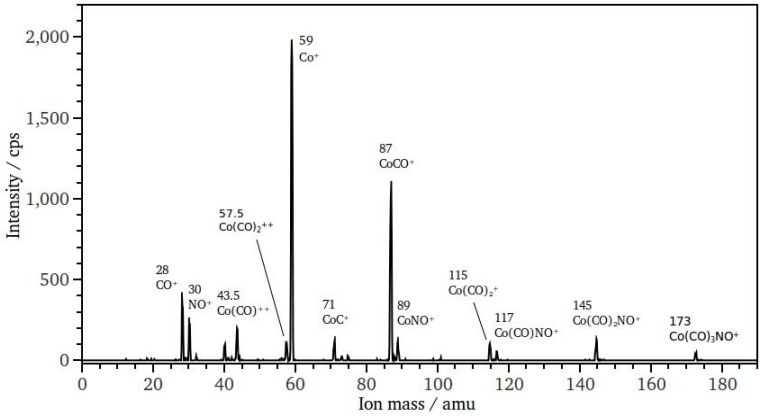

Fig.1. Mass spectrum of $Co(CO_3)NO$ with the corresponding positive ionic products reported.

Acknowledgments: This work was supported by the Slovak Research and Development Agency, project Nr. SK-SRB-0011-09. Financing of this work was by the Slovak Grant Agency VEGA-1/0558/09 and from the COST ECCL project.

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Near-threshold electron-impact ionization of thymine

I. V. Chernyshova, J. E. Kontros, P. P. Markus, O. B. Shpenik

Institute of electron Physics, Ukrainian National Academy of Sciences
21 Universitetska str. Uzhgorod 88017, Ukraine

The main mechanisms of destruction of living cells by ionizing radiation can be studied in collisions of biomolecules with slow electrons. Thymine belongs to pyrimidine nucleobase playing an important role in the vital functions of living organisms.

Below the results of investigations of electron-impact ionization cross section of thymine molecule is presented. Experiment was performed using a modernized hypocycloidal spectrometer with energy resolution not exceeding 0.3 eV [1]. The molecules were produced using a compact effusion source made of the stainless steel. The temperature of the gas-filled cell was taken about 10 K higher than that of the molecular vapor in the heated reservoir. The electron energy scale was calibrated using the position of the maximum of the first derivative of the electron beam current in the initial area of the voltage-to-current characteristic.

In Fig.1, the total electron-thymine molecule ionization cross-section in the energy range from the threshold up to 16 eV is presented. The first ionization potential (IP) stated by us is equal to 9.12 eV. Detailed analysis of the measured ionization curve allows the number of weak features related to the appearance of fragment ions of the investigated molecule to be found. It was obtained 4 appearance energies (AE) equal to 10.03, 10.37, 10.87 and 12.24 eV, respectively. The obtained values of the ionization potentials coincide well with experimental and calculated ones in [2].

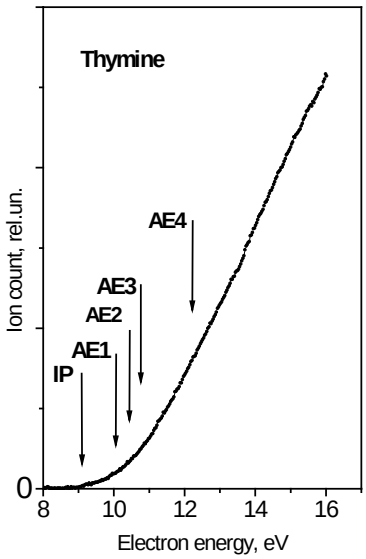

Fig.1. The total electron-thymine ionization cross-section.

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Positive and negative electron-impact ionization of the cytosine molecule

I. V. Chernyshova, J. E. Kontros, P. P. Markush, O. B. Shpenik

Institute of Electron Physics, Ukrainian Academy of Sciences, 21 Universitetska str. 88017 Uzhgorod, Ukraine
E-mail: gzav@gmail.com

The cytosine molecule (Cy) is one of the four nucleic acid bases involved in the DNA molecule composition, which plays an essential role in living activity of the live organisms, therefore, the comprehensive studies of the properties of this molecule are of great importance. Here we report on the results of our studies on the total cross sections for the production of both positive and negative ions of the cytosine molecule at the collisions with slow (E<30 eV) electrons.

In our experiment, the hypocycloidal electron monochromator [1] was used to produce an electron beam with the energy resolution not worse than 0.2 eV. The cytosine powder (99%, Aldrige product) placed into the quartz ampoule was heated up to ~100°C temperature in the stainless-steel reservoir. The target was formed in the gas-filled cell conditions (P»10^{-3} Torr). The ions produced were extracted to the collector mounted perpendicularly to the ion beam direction. A grid (of the 80% transparency) was placed in front of the collector. A low negative potential was applied to the collector when detecting the positive ions, while for the negative-ion detection its polarity was changed to the positive one.

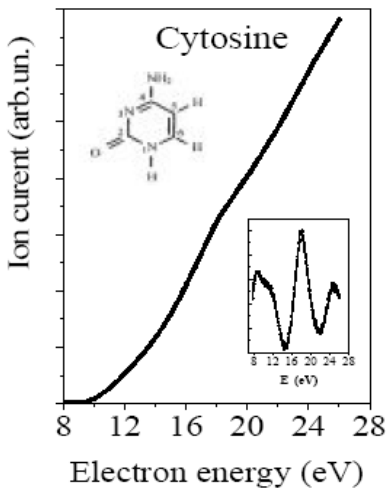

Fig.1. Total electron-impact ionization cross section for the cytosine molecule.

Figure 1 shows the total ionization cross section for the Cy molecule within the energy range from the threshold up to 26 eV. The molecular Cy^+ ion appearance energy was determined to be Ei = 8.82 ± 0.05 eV. The thorough measurements allowed the weak features in the ionization curve to be observed being related to the production of the ionic fragments of the initial molecule. The most prominent features of the cross section are observed at 18.1 eV and 24.58 eV energies (see inset in Fig. 1). The first one is related to the electron excitation from the 9a (σ) and 8a (σ) molecular orbitals with binding energies lying from 17.30 to 19.70 eV [2]. The second feature could be assigned to the involvement of the double ionization process of the Cy molecule predicted in [3]. An intense structure in the total negative ion yield cross section (with a maximum at 1.54 eV) was observed by us in the 0–4 eV energy region. As the mass spectrometricstudies [4] have shown, this structure is due to the $(Cy\text{-}H)^-$ negative ion formation via the electron dissociative attachment to the initial molecule. Above 4 eV the shape of the cross section is determined by the total contribution of the $(C_3H_3N_2)^-$, $(C_3HN_2)^-$, $(OCN)^-$, and $(CN)^-$ fragment anions.

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Electron impact excitation of the gas-phase thymine molecule

M. M. Erdevdy, O. B. Shpenik, V. V. Zvenihorodsky

Institute of Electron Physics, Ukr.Nat.Acad.Sci., 21 Universitetska str., 88017 Uzhgorod, Ukraine

The studies of the processes taking place in biomolecules at their interaction with low-energy charged particles allow the role of excited states to be traced on the initial stages of biological processes. Under electron impact the nucleic base molecules undergo different elementary processes: excited state formation, ionization, fragmentation and dissociative electron attachment. Experiments on the model systems, i.e. pyrimidine base, enable the processes occurring in the living cell to be understood.

Here we report on the results on the thymine ($C_5H_6N_2O_2$) molecule excitation by slow electrons. Experiment was carried out using the gas-filled cell at the incident electron current of 7 – 10 μA (the energy spread being 0.5 eV (FWHM)) provided by a triode gun with an oxide cathode. The optical emission due to electron impact was separated by a diffraction monochromator and detected by a photomultiplier. An automated setup and measuring technique are described in [1]. Figure 1 shows the emission spectrum of the thymine molecule measured at the 15, 30, 50, 70 and 100 eV electron energies. A number of low-intensity emission bands are observed in the 280 - 500 nm region with the maxima at 289, 309 - 315, 336, 359, 386, 397, 410, 434 and 487 nm. The 386 nm band could result from the CN (the $B^2\Sigma - A^2\Pi$ transition) and the CNC group emission (the $\Delta^2 - {}^2\Pi$ transition). The NH_2 band may also contribute to the above band formation. The 336 and 359 nm bands could result from the NCN (the ${}^3\Pi_u - {}^3\Sigma_{g^-}$ transition) and HNCN group emission (the $\tilde{A} - X\square$ transition). The 434 nm band could result from a superposition of the CH (the $A^2\Delta - X^2\Pi$ transition) and N_2CH_2 group emission (the $\tilde{A} - X\square$ transition).

Figure 2 shows the optical band excitation functions (OEFs) for the different band shapes. For example, the excitation functions for the band λ_{max}=336 nm and λ_{max}=359 nm where measured with the 400 meV energy step. As seen, these functions have different characteristics and structural features.

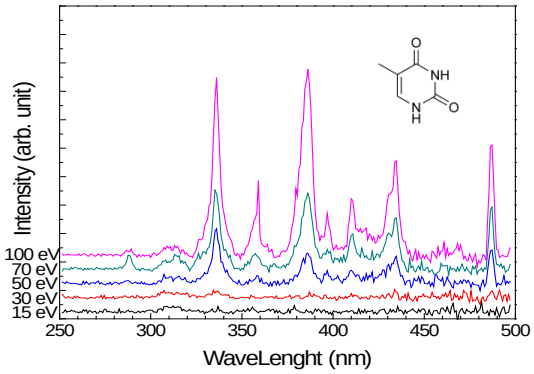

Fig.1. Thymine molecule emission spectrum.

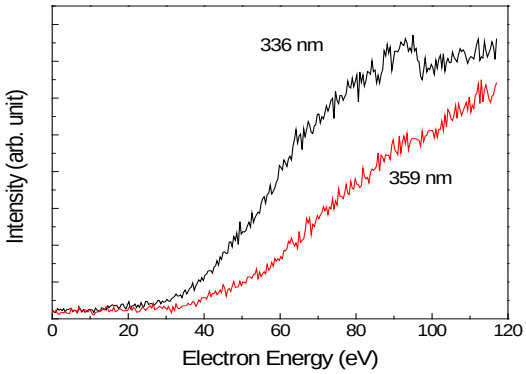

Fig.2. OEFs of spectral bands at 336 and 359 nm.

One may conclude that the experimental approach used in this study made it possible to obtain new data on the electron impact excitation of the thymine molecule.

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Electron impact excitation of the gas-phase uracil molecule

O. B. Shpenik, M. M. Erdevdy, V. V. Zvenihorodsky

Institute of Electron Physics, Ukr.Nat.Acad.Sci., 21 Universitetska str., 88017 Uzhgorod, Ukraine

The problem of studying the processes in biomolecules under the low-energy impact is crucial in tracing the course of biological processes. In this case the nucleic base molecules undergo a number of physical processes: excitation, ionization, fragmentation etc. The above studies with such model systems as pyrimidine base allow the processes in the living cell to be analysed.

Here we report on the results on the uracil ($C_4H_4N_2O_2$) molecule excitation by slow electrons. Experiment was carried out using the gas-filled cell at the incident electron current of 7 – 10 μA (the energy spread being 0.5 eV (FWHM)) provided by a triode gun with an oxide cathode. The optical emission due to electron impact was separated by a diffraction monochromator and detected by a photomultiplier. An automated setup and measuring technique are described in [1]. Figure 1 shows the emission spectrum of the uracil molecule measured at the 25, 40, 60 and 100 eV electron energies. A number of low-intensity emission bands are observed in the 280 - 500 nm region with the maxima at 290, 309 - 317, 338, 360, 388, 430 and 490 nm, as well as one extremely intense band with the maximum at 388 nm. This band could result from the CN (the $B^2\Sigma - A^2\Pi$ transition) and the CNC group emission (the $\Delta^2 - {}^2\Pi$ transition). The NH_2 band may also contribute to the above band formation. The 338 and 360 nm bands could result from the NCN (the ${}^3\Pi_u - {}^3\Sigma_{q-}$ transition) and HNCN group emission (the Ã – X□ transition). The 430 nm band could result from a superposition of the CH (the $A^2\Delta - X^2\Pi$ transition) and N_2CH_2 group emission (the Ã – X□ transition).

Figure 2 shows the optical band excitation function (OEFs) for the different band shapes. For example, the excitation functions for the band λ_{max}=338 nm and λ_{max}=388 nm where measured with the 400 meV energy step. As seen, these functions have similar characteristics and structural features.

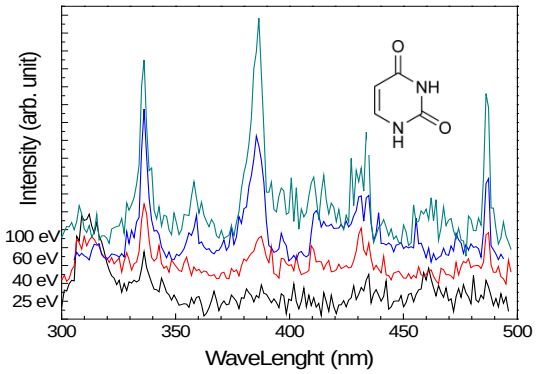

Fig.1. Uracil molecule emission spectrum.

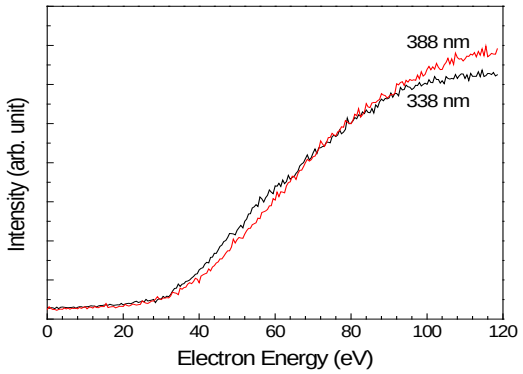

Fig.2. OEFs of spectral bands at 338 and 388 nm.

One may conclude that the experimental approach used in this study made it possible to obtain new data on the electron impact excitation of uracil molecule.

REFERENCES

[1] N.M.Erdevdi, O.B.Shpenik and V.S.Vukstich. Precision measurements of optical excitation function for the mercury atom, Opt.Spectrosc. 95(4) (2003) 529-536.

Site-selective fragmentation studies of halogenated pyrimidines in the valence and inner shell region

M. C. Castrovilli[a,b], P. Bolognesi[a], P. O'Keeffe[a], A. Casavola[a], D. Catone[c], S. Turchini[c] and L. Avaldi[a]

[a]*CNR-IMIP, Area della Ricerca di Roma 1, Monterotondo Scalo, Italy*
[b]*Dipartimento di Chimica "G. Ciamician", Università di Bologna, Bologna, Italy*
[c]*CNR-ISM, Area della Ricerca di Roma 2, Roma, Italy*

Gas phase studies of isolated, small biomolecules provide relevant information on the properties of the basic units of a biological system in an environment free from interactions. Here the halogenated pyrimidines, which are analogues of pyrimidine, have been investigated for their potential application as radiosensitisers in radiotheraphy. Indeed their incorporation into the DNA of a tumor cell makes the irradiated cells more sensitive to double strand breaks (DSB) [1,2], because the response of the halogenated compounds to radiation damage changes drastically with respect to the unsubstituted pyrimidine bases. We have studied at the GAPH and CIPO beamlines of the Elettra Synchrotron radiation source, Trieste (Italy), the selective molecular fragmentation of pyrimidine and some halogenated pyrimidine molecules (figure 1) induced by the absorption of VUV/soft X-ray radiation to understand this effect.

We have investigated the valence dissociation via the measurement of the fragments appearance energy (AE) by mass spectrometry. The experimental data have been compared with the results of a computational analysis. The AEs have been extracted by the partial ion-yields, at a fixed value of m/z, over the range 9-15 eV and calculated at the G3B3 and B3LYP levels of theory. In all the studied molecules the fragment m/z=52, due to loss of HCN and the halogen atom has been observed. In figure 2 the partial ion yields for this fragment in 5-Br- and 2-Br-pyrimidines are shown. The differences in the observed AEs can be related to the position of the halogen atom.

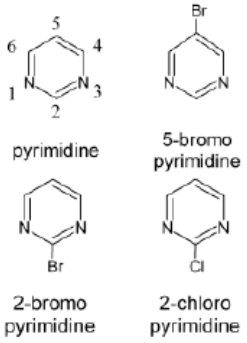

Fig.1. Pyrimidine and halogenated pyrimidines.

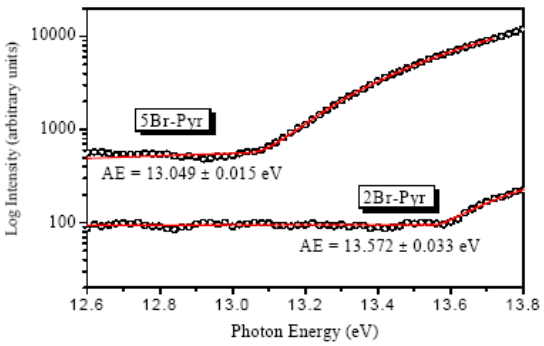

Fig.2. Partial ion yield of $C_3H_2N^+$ (m/z=52) fragment. The full curve is a fit with a modified Wannier threshold law.

In the inner shell region, the fragmentation patterns have been observed to be significantly dependent on the atomic site of the energy deposition, selected via suitable choice of the photon energy for inner-shell resonant excitation. Electron-ion coincidence experiments combined with theoretical characterization have allowed us to explain this observation in pyrimidine.

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Calculations of the structure and photoionization processes of pristine and endofullerenes

A.V. Verkhovtsev[a], R.G. Polozkov[a], V.K. Ivanov[a], A.V. Korol[b], A.V. Solov'yov[b]

[a] *St. Petersburg State Polytechnic University, St. Petersburg, Russia*
[b] *Frankfurt Institute for Advanced Studies/Goethe University, Frankfurt am Main, Germany*

The results of many-body theory calculations of electronic structure and photoionization cross sections for the fullerene C_{60}, its ions and noble gas endohedral fullerenes are presented. The valence 240 electrons of the fullerene are distributed in a usual way with the ratio of 3:1 over the σ (none-node) and π (one-node) orbitals correspondingly. The fullerene ionic core is described by a uniform distribution of positive charge (Z=240) over a spherical layer of finite thickness [1].

The single-electron energies and wave functions of 240 valence electrons in C_{60} are determined from the solution of the system of self consistent Hartree-Fock (HF) equations with the jellium-like spherically symmetric field of the ionic core. The total electronic system of endohedral fullerene consists of all the electrons of encapsulated atom and 240 valence electrons of the fullerene C_{60}. All the electrons are treated again within the HF approximation with the spherically symmetric field of the ionic core and the point nuclear charge of the embedded atom placed at the center of the system. The concrete calculations are performed for the $He@C_{60}$, $Ne@C_{60}$, $Ar@C_{60}$, $Kr@C_{60}$ and $Xe@C_{60}$ compounds. The analysis of electron density distributions reveals the strong hybridization of atomic outer-electron states and the corresponding states of the fullerene shell. Because of that a part of the electron density is transferred from the encapsulated atom to the outer fullerene shell. This creates the negatively charged fullerene layer surrounding the embedded ion. Note the HF results on the electron density distributions in endofullerenes differ significantly from the LDA results reported in [2].

The discrete and continuum spectra wave functions of the above systems are obtained in the frozen-core HF approximation. These wave functions are used to calculate the HF dipole amplitudes and photoionization cross sections. The amplitudes and cross sections, in which the many-electron correlations are accounted for, are derived within the Random Phase Approximation with Exchange (RPAE). The calculations of the fullerene C_{60} photoionization process reveal two maxima in the total cross section due to the appearance of the two collective plasmon excitations, the so-called symmetric and anti-symmetric surface plasmon modes. The comparison of the HF and RPAE results demonstrate the extremely important role of many-electron correlations in the photoionization processes considered. For the endohedral fullerenes the partial cross sections exhibit the oscillatory behavior due to the interference of the outgoing electronic waves [3,4]. This behavior is sensitive to the electron density distribution of the embedded atom and fullerene shell.

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Major and trace elements in mouse bone measured by surface and bulk sensitive methods

I. Benkő[a], I. Rajta[b], A. Csik[b], J. Tóth[b], K. Géresi[a], É. Ungvári[a],
B. Szabó[c], G. Sarkadi[b], and K. Tőkési[b]

[a]*Department of Pharmacology and Pharmacotherapy, Medical and Health Science Center, University of Debrecen, Hungary*
[b]*Institute o f Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary*
[c]*Heart Center, Semmelweis University, Budapest, Hungary*

In the past years an increasing research interest turned to the accurate determination of the components of the bone samples. These investigations focused on both the major and trace elements in the bone. Work in this field is strongly motivated because the accurate knowledge of various major and trace element concentrations can be a good indicator of the detection of several diseases. Also important to note that bones can be one of the final destination in the body where toxic elements can be deposited.

The aim of the present work is to investigate the major and trace elements in the mouse bone. We take the advantage of our institute (ATOMKI) that we have number of techniques available for these studies. We used the followings: Particle induced x-ray emission (PIXE), X-ray photoelectron spectroscopy (XPS), Secondary Neutral Mass Spectroscopy (SNMS), and Scanning Electron Microscope (SEM).

The bone samples were prepared in the Medical and Health Science Center of the Debrecen University. We used femurs of the mouse in our studies. The bone marrow was washed out with distilled water many times through a fine needle syringe. Then the bones were dried for a day and one of the femurs of the mouse was used for analysis in this natural form (see Fig. 1). The other femurs of each mouse were calcinated to prepare bone powder.

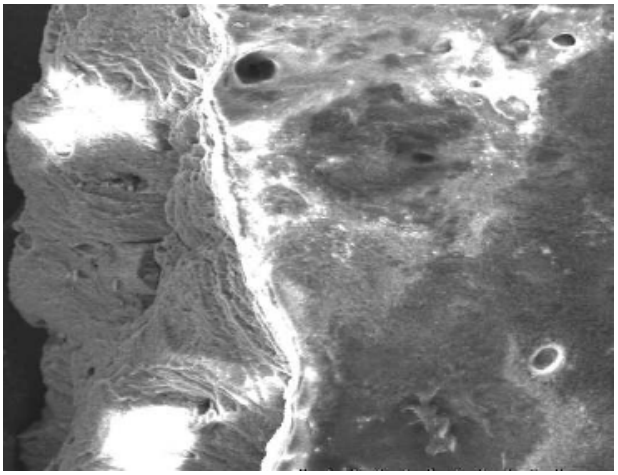

Fig.1. Scanning electron microscope image of the mouse bone before calcinations.

We show concentration profiles for various major and observable trace elements of the mouse bone. We present critical analysis of our data in comparison with other results.

Acknowledgments: The work was supported in part by the Hungarian Scientific Research Fund OTKA Nos. K67873, K72172, K73703 and by cost action No. MP1002.

Influence of the environment on the fragmentation of amino acids provoked by low-energy ions

S. Maclot[a], M. Capron[a], R. Maisonny[a], E. Lattouf[a], A. Ławicki[a], S. Bari[b], A. Méry[a], J. Rangama[a], J.-Y. Chesnel[a], A. Domaracka[a], J.-C. Poully[a], R. Hoekstra[b], T. Schlathölter[b], B. Manil[c], L. Adoui[a], P. Rousseau[a], B. A. Huber[a]

[a]*CIMAP, CEA/CNRS/ENSICAEN/Université de Caen Basse-Normandie, Boulevard Henri Becquerel, F-14070 Caen, France*
[b]*KVI, Atomic and Molecular Physics, University of Groningen, Zernikelaan 25, Groningen, NL-9747AA, The Netherlands*
[c]*LPL, CNRS/Université Paris 13, Institut Galilée, 99 Avenue J. B. Clément, F-93430 Villetaneuse, France*

The objective of the present experiments is to study ion-induced fragmentation of biomolecules, more particularly amino acids. These molecules are essential for life, and they fulfill many important functions in metabolism. They are the building blocks of proteins, which are chains of amino acids.

An improved understanding of the cleavage of these molecules could give better insights into radiation damages occurring in biological tissues [1] for example in the case of hadrontherapy. Furthermore, the interaction of solar wind or cosmic rays with tails of comets could play an important role for the creation of first prebiotic molecules.

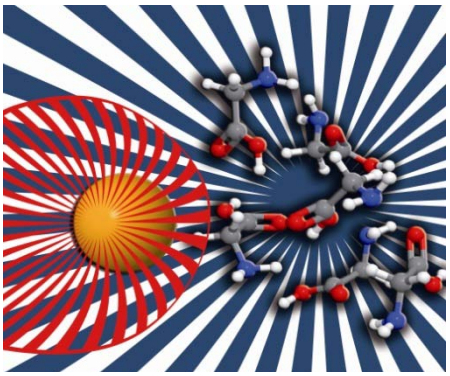

Fig.1. Artistic view of the collision between a projectile and a glycine hexamer.

In the present contribution, we will consider the fragmentation of two amino acids in the gas phase: glycine (NH_2CH_2COOH) and valine ($(NH_2)(CH_3)_2(CH)_2COOH$) upon their interaction with multiply charged ions (Xe^{20+} at 300 keV). Products of the interaction are analysed by time-of-flight mass spectrometry. Gas phase production of biomolecules is performed using an oven. Two different cases will be discussed: the isolated molecule and clusters of amino acids. The differences between both measurements and the influence of the environment on the fragmentation behaviour will be examined.

In general, radiation-induced fragmentation of small amino acids is governed by the cleavage of the C-C_α bond, the backbone of the molecule [2]. Embedding the molecule in clusters changes the fragmentation pattern. Peaks due to pathways involving the cleavage of the C-C_α bond are strongly reduced and some even disappeared. There is an effect of the environment on the fragmentation [3]. Amino acid clusters are hydrogen-bonded networks of amino acid monomers. The excess energy is redistributed within the cluster which causes the hydrogen bond which is the weakest bond in the system to break preferably. The remaining internal energy is too low to induce intramolecular fragmentation.

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A specific beamline at a 5 MV electrostatic accelerator for studying ion-biomolecule collisions in the energy region of the Bragg peak

S. Kovács[c], P. Herczku, Z. Juhász, L. L. Horváth, F. Gáll[+], B. Sulik

Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Bem tér 18/c, H-4026 Debrecen, Hungary.

In the past decades, considerable effort has been devoted to study atomic collisions in a wide range of impact energies and collision partners. Today, we understand the basic mechanisms and the most important collision scenarios (see e.g., [1] for electron emission). Due to the refined experimental methods, higher order processes have became routinely observable, and kinematically complete experiments can be performed providing fully differential cross sections. There is an increasing demand from the side of applications to utilize the results of the fundamental atomic collision research. At this point, we often face with the lack of sufficient knowledge about relevant processes, though similar systems and processes have already been investigated. A good example for this is cancer therapy by energetic ion impact, where e.g., the energy deposition is important, but not the most relevant quantity [2]. For optimizing the efficiency of the therapy, a multitude of collision mechanisms should be carefully considered in a wide impact energy range.

Here we report about a specific beamline for fundamental research on atomic and molecular collisions according to the demands of applications related to radiation damages. We focus on mechanisms which may significantly enhance the fragmentation yield of biomolecules (from water to DNA) by ion impact around the maximum and at the low energy side of the Bragg peak, by experiments in the ion energy range of 50-1000 keV/u at the beamline of the VdG-5 accelerator in Atomki, Debrecen.

The beamline consists of a 15^{o} electrostatic deflector chamber for the projectile ions, and a magnetically shielded universal experimental chamber of 1 m diameter. The electrostatic deflection is advantageous for heavier ions, and it also offers an easy way to chop the beam for time of flight experiments. In the chamber, there are two rotatable rings with angular calibration. The high vacuum system assures a background pressure of 10^{-7} mbar. The main target is an effusive molecular gas jet which is designed for these experiments. The target gas density can be varied from $7\cdot 10^{12}$ 1/cm^3 to $1\cdot 10^{14}$ 1/cm^3 with a set of wads and nozzles. We developed a specific electrostatic spectrometer which is able to measure in the 15° - 165° observation angle range relative to the beam direction. This is a 45° parallel plate spectrometer, which can be used up to E/q=10 keV. The spectrometer is equipped with an electrostatic lens for acceleration and deceleration. Time of flight spectrometers are under construction. We would like to measure double differential cross section of molecular fragments (both cations and anions) with and without coincidence conditions. Preliminary results from the first measurements are planned to be displayed at the conference.

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[c] kovacss@atomki.hu

[+] deceased

Oscillations in the Auger energy distribution following atoms colliding with molecules

B. S. Frankland[a], R. O. Barrachina[b], J.-Y. Chesnel[a], F. Frémont[a]

[a]*CIMAP, Unité Mixte Université de Basse-Normandie CEA-CNRS-Ensicaen, 6 bd Mal Juin, F14050 Caen Cedex France*

[b]*Centro Atómico Bariloche and Instituo Balseiro (Cómision Nacional de Energía Atómico and Universidad Nacional de Cuyo), 8400 S.C. de Bariloche, Río Negro, Argentina*

In 2004, a novel Young-type experiment was proposed and studied theoretically by Barrachina and Zitnik [1]. The collisional process can be summarized as follows:

$$He^{2+} + H_2 \rightarrow He^{**}\left(2\ell 2\ell', n \geq 2\right) + H^+ + H^+$$

where the outgoing autoionizing helium plays the role of the source of single-electron, while the two residual protons provide the double-center interferometer.

Oscillations in the angular distribution of the autoionization intensity could be observed (open circles in Fig. 1) at angles in the range 90°-170° [2]. The theoretical interpretation of this result is not straightforward for several reasons. First, the autoionization process depends on the double capture process. In addition, autoionization is affected by the post-collisional interaction due to the presence of the proton, creating a distortion of the energy and angular distributions of the emitted electron.

Barrachina and Zitnik calculated, using a Final State Interaction model [1], the autoionization probability for the configuration $2s^2\ {}^1S$ by using a peaking approximation. Their results show that the autoionization intensity presents oscillations on the angular distribution due to Young-type interferences.

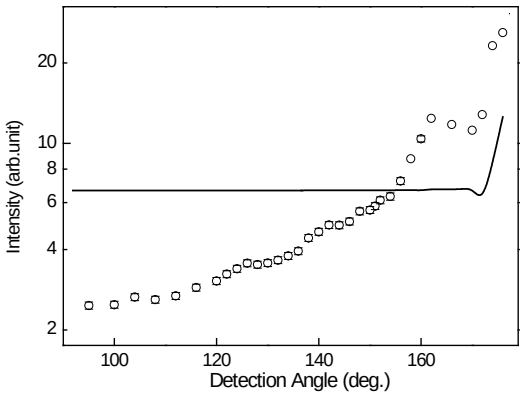

Fig.1. Total intensity for autoionization following double capture in 30 $keV\ He^{2+} + H_2$ collisions, as a function of the detection angle. Open circles ; experimental result. Solid line ; theoretical result.

We improved the study by avoiding this approximation. Surprisingly, the expected oscillations due to Young interferences are absent in the calculated angular distribution (Fig. 1). Nevertheless, a Fast Fourier transform analysis reveals frequency structures corresponding to a period of ~14° that are not visible in the case of He^{2+} + *He* collisions. The results will be discussed in details during the conference.

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Spatial resolution test of a beam profile monitoring system with a proton beam of energy 0.5, 1, 10, and 40 keV

S. Das[a], A. Källberg[a], and J. Harasimowicz[b]

[a]*Manne Siegbahn Laboratory, Department of Physics, Stockholm University, Stockholm, Sweden*
[b]*Department of Physics, University of Liverpool, UK and Cockcroft Institute, Daresbury, UK*

Beam profile monitoring system (BPMS) is an essential part of any beam diagnostics [1]. A BPMS based on the observation of low energy secondary electrons (SE) generated by a beam striking a metallic foil was recently developed by Kruglov et al [2].

Inspired by its simplicity and applicability, a similar BPMS to cover the wide range of beam intensities and energies was built at Stockholm University for the DESIREE (Double ElectroStatic Ion Ring ExpEriment) beam line diagnostics [3]. It consists of an aluminum (Al) plate, a grid placed in front of Al, a microchannel plate (MCP), a fluorescent screen (F.S.), a PC, and a CCD camera. A beam collimator containing a set of circular holes of different diameters and separation between them was built to check the spatial resolution of the system. Two holes of diameter 1 mm each and separated by 2 mm in the collimator and a proton beam of energy 0.5, 1, 10, and 40 keV, respectively, were used for the measurements. From the entire beam the collimator cuts out well separated and approximately same intensity two beam spots. After passing through the collimator, the beam strikes the Al plate and produces a lot of SE. These SE are then first accelerated to the grid and then hit the MCP where they get amplified. The cascade of electrons from the MCP then hits the F.S. and produces flashes of light, which are, in turn, captured by a CCD. This CCD is connected to a PC for further storage and analysis of the recorded light intensities.

The resolution of the system was tested for different Al plate voltages. From Fig. 1 (i - iii) two circular images of approximately same diameter (~ 1 mm) with a separation of 2 mm between the beams centers can be clearly seen for 10 keV proton beam, suggesting a spatial resolution of 2 mm of the system. Fig. 1 (iv) shows the corresponding horizontal beam profile of Fig. 1(i). The change of resolution [represented by the ratio $\delta = \{(a+b)/2-c\} / (a+b)/2]$ of the BPMS was calculated from the horizontal beam profile and was found to increase with increasing Al plate voltage (Fig. 2).

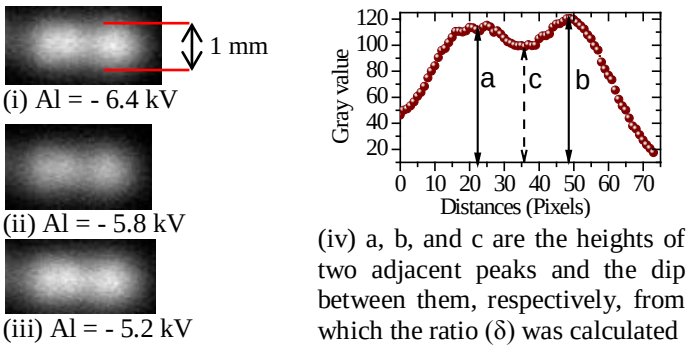

Fig. 1. Recorded CCD images (i - iii) (MCP = 1100 V, F.S. = 4945 V). (iv) shows the horizontal beam profile of image (i).

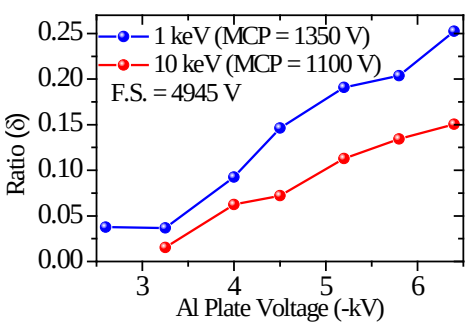

Fig. 2. Change of resolution (Ratio δ) vs. Al plate voltage for 1 and 10 keV proton beam.

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Radiative electron capture and K-shell vacancy production in ^{32}S, ^{35}Cl + Cu collisions at 0.5 ÷ 2.5 MeV/u energies

A. C. Scafes, C. Ciortea, D. E. Dumitriu, A. Enulescu,
D. Fluerasu, M.M. Gugiu, D. M. Pena and I. Piticu

Department of Nuclear Physics, National Institute for Physics and Nuclear Engineering "Horia Hulubei" (IFIN-HH), P.O. Box MG-6, Magurele, jud. Ilfov, 077125 Romania

The purpose of the present work was to determine K-shell radiative electron capture and ionization cross sections for two collision systems, ^{32}S, ^{35}Cl + Cu, at 0.5-2.5 MeV/u energies. Integral X-ray yields of both collision partners, in experiments performed at the Tandem accelerator of IFIN-HH, have been measured. For determination of the cross sections from the measured X-ray yields, multiple ionization of the outer shells have been taken into consideration, and using the X-ray energy and yield shifts method [1] the outer-shells mean ionization probabilities per electron have been estimated.

Different excitation mechanisms, direct ionization [2], radiative electron capture [3] and molecular orbital excitations [4] are discussed. Comparison of the experimental data with model calculations will be presented.

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Chemi-ionization processes in slow Neon Rydberg atom collisions with ground state parent atoms

A. A Mihajlov [a], V. A. Srećković[a] , Lj. M. Ignjatović[a]

[a]*Institute of Physics, University of Belgrade, P.O. Box 57, 11001 Belgrade, Serbia*

In the presented work possibilities have been investigated of describing chemi-ionization processes in atom-Rydberg atom collisions involving atoms with multiple electrons in their outer (valent) shell on the base of so-called dipole resonance mechanism. Therefore, the processes of Penning and associative ionization have been considered: $Ne^*(n) + Ne \Rightarrow Ne + Ne^+$ and $Ne^*(n) + Ne \Rightarrow Ne_2^+$, where the principal quantum number $n >> 1$, for which the effective cross-sections and the rate coefficients have been determined at temperatures T=300K and 600K.

The calculations were carried out using adequately modified methods which had been worked out earlier in the context of chemi-ionization processes in alkali, helium, and hydrogen plasmas [1,2,3]. The results of the calculations were then compared with the existing experimental results. It has been shown that the methods developed provide good determination of the effective cross-sections and rate coefficients for the considered processes in the low-temperature region.

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Effects of 200 keV argon ions irradiation on microstructural properties of titanium nitride films

M. Popović[a], M. Novaković[a], N. Bibić[a]

[a]*VINČA Institute of Nuclear Sciences, 11001 Belgrade, Serbia*

This paper reports on a study of microstructural changes in TiN/Si bilyers due to 200 keV Ar^+ ions irradiations at room temperature. The 240 nm TiN/Si bilyers were prepared by d.c. reactive sputtering on crystalline Si(100) substrates. The irradiated ion fluencies were in the range from $5x10^{15}$ ions/cm^2 to $2x10^{16}$ ions/cm^2. Structural changes in the TiN/Si bilyers were analysed by Rutherford Backscattering Spectroscopy (RBS), X-ray diffraction analyses (XRD) and Transmission Electron Microscopy (TEM). The irradiations caused the microstructural changes in TiN layers, but no amorphization even at the highest argon fluence of $2x10^{16}$ ions/cm^2. More precisely, the irradiations resulted in variation of lattice constants, micro-strain and grain size of the TiN films [1], [2].

Figure 1 shows high resolution image in cross section taken from the sample irradiated to $2x10^{16}$ ions/cm^2. It can be observed that the interplanar distances are fully consistent with the TiN phase.

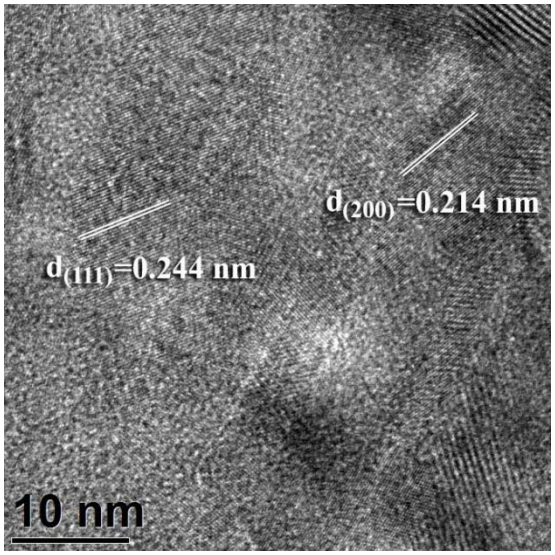

Fig.1. High resolution image in cross section of the sample irradiated with 200 keV argon ions to $2x10^{16}$ ions/cm^2

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Elementary processes of interaction of slow electrons with metal surfaces

O.B. Shpenik[a*], T.Yu. Popik[a], R.O. Ortikov[a], V.M. Feyer[b], Yu.V. Popik[c]

[a]*Institute of Electron Physics, Ukrainian Academy of Sciences, 21 Universitetska str., 88017 Uzhgorod,Ukraine*
[b]*Sincrotrone Trieste, Area Science Perk, I-34012 Basovizza (Trieste), Italy*
[c]*Uzhhorod National University, Voloshina Str., 54, 88000 Uzhhorod, Ukraine*
[*]*E-mail: gzav@gmail.com*

Using the technique of slow (0–10 eV) monoenergetic (FWHM 50–100 meV) electron backscattering spectroscopy, elementary processes of interaction of slow electrons with metal surfaces are studied. A variety of objects were studied: Au, Ag, Pt, Cu, W, Ta, Mo polycrystalline surfaces as well as Mg and Bi films evaporated on different substrates [1]. The experiments were performed for both atomically clean surfaces as well as at different exposures of the surfaces to the residual gas atmosphere at pressures from 10^{-8} to 10^{-6} Pa.

We studied the energy dependences of elastic electron backscattering intensity; energy loss spectra at different primary electron energies; constant residual energy spectra: energy dependences of slow electron total scattering intensities; angular dependences of the scattered electrons at different incident beam energies.

The characteristics under investigation are shown to be very sensitive to the chemical purity of the surface under study (atomically clean or covered with residua gas atoms). The analysis of the experimental results obtained as well as the known theoretical calculations of the band structure of the metals under study enables one to conclude that the fine structure observed in the experimental dependences is related to the excitation of electron states. The features being revealed are assigned to the energy transitions between the maxima of densities of filled and empty electron states in the valence and conduction bands of the reduced Brillouin zone.

The features in the spectra, dependent of the surface state, with the energies not matching the electron transitions in the bulk, are related to the excitation of surface electron states. For Mo and W surfaces, exposed to the residual gas atmosphere at 10^{-7} Pa for several hours, a structure is revealed whose shape and energy position corresponds to the $^2\pi_g$ resonance state of nitrogen molecule.

The results obtained are in a good agreement with the known experimental data obtained by ultraviolet electron spectroscopy, X-ray photoelectron spectroscopy, photoabsorption, characteristic energy loss spectroscopy and with theoretical calculations of the band structure of the objects under study and essentially complement these data.

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Investigation of MeV proton microbeam transmission between two flat plates – the cases of homogeneous metallic and insulator plates

I. Rajta, R. J. Bereczky, K. Vad, and K. Tőkési

Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary

During the last decade a continuous interest is put in an appearance for the study of charged particles interactions with cylindrical surfaces based on various capillary targets from nano- to macrometer size. The main reason of the first investigations belonged to the fundamental research interest for deeper understanding of ion and metallic surface interactions. However, due to the discovery of the unexpected effect of charged particle guiding using insulator capillaries, the main interest later focused onto the investigation of the interaction between ions and insulating samples. In contrast to the case of metallic capillaries, the experiments with insulating ones showed that the ions keep their initial charge state even if the capillary axis was tilted compared to the beam axis, in such a way that the ions had to hit the wall. The obtained particle guiding is a direct consequence of a self-organized charge-up process inside the capillary. We have shown that the guiding effect known from nanocapillaries is also valid up to macroscopic dimensions of the order of mm [1].

Along this line, in this work we did further simplification, and instead of cylindrical shape target we used flat plates. The length of the plates was L=20 mm, and the distance between the two plates, i.e. the air gap, was around d=170 μm. We prepared two identical samples. In both cases glass plates were used and one pair of plates was covered by a few nm thick gold layer. So the possible differences and commonalities of particle transport through metallic and insulator plates can be studied. We performed the measurements with a 1 and 2 MeV proton beam. The beam spot size was 1 μm, with a beam current of about 1000 proton/s, and the angle of the beam divergence was less than 0.07 °. The axis of the plates, at the beginning of the measurement, was aligned to the direction of the proton microbeam.

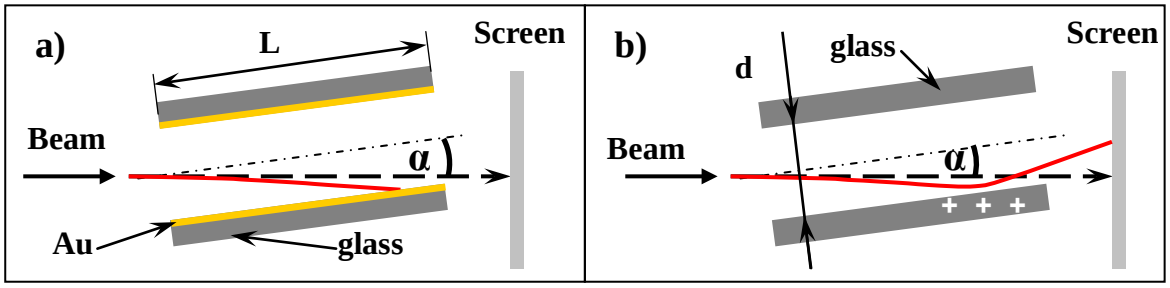

Fig.1. Schematic diagram of our samples with the expected proton trajectory (solid red line): a) metallic plates, b) insulator plates.

Acknowledgments: This work was supported by the Hungarian Scientific Research Fund OTKA Nos. K72172, K83886.

We present results of the transmitted proton intensities measured as a function of the tilt angle α for both metallic and insulator plates. α is the angle between the beam axis and the axis of the plates. We will also show results for the distance-dependent features of the particle transport, because the providential combination of our target with the proton microbeam allows us this investigation.

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Ion-guiding and blocking of ion transmission in dense polycarbonate nanocapillary arrays at 3 keV Ar^{7+} impact

Z. Juhász, P. Herczku[c], S. Kovács, R. Rácz, S. Biri, I. Rajta, G. Gáll, S. Szilasi and B. Sulik

Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Bem tér 18/c, H-4026 Debrecen, Hungary.

The guided transmission of ions through nanocapillaries has received a great deal of attention in the past decade. Ions can be guided in insulating capillaries by the electric fields created by charging up the capillary walls [1]. Recently, the formation and dynamics of charge patches was studied in details for nanocapillaries in polyetilene terephtalate (PET) and polycarbonate (PC) foils [2-4]. For the studied PC samples, the capillary density was tipically low (10^6 – 10^7 capillaries per cm^2). In such cases, the charge which is accumulated in one capillary does not alter significantly the electric field of the neighboring capillaries.

In the present work we study the dynamic properties of guiding of 3 keV Ar^{7+} ions through nanocapillaries created in PC with high density. We used commercially available filter foils with a density of $4 \cdot 10^8$ capillaries per cm^2. The capillary diameter was 170 nm. The length of the capillaries (i.e., the foil thickness) was 30 μm. The intensity and the angular distribution of the transmitted ions were studied by measuring the two-dimensional transmission profiles with a position sensitive channel plate detector system. Ions and neutrals were separated by electrostatic deflection. The temporal evolution of the transmission was studied as a function of the charge deposited on the sample surface.

The tilt angle of the capillary axis was varied from 0° to 7°. The mean emission angle of the transmission profiles exhibit weak oscillations. Similarly to earlier PC studies for low density samples [3], at high density we also observed the decrease of the profile intensities with irradiation time, providing evidence of blocking effects on the ions which is probably due to a repulsive field produced by charge deposition inside the capillaries. In addition, in the present work the intensity of neutrals has also been measured. Their intensity found to be decreasing with the collected charge, while, the ratio of neutrals to ions was increasing. Detailed analysis will be provided at the conference.

Acknowledgments: This work was supported by the Hungarian National Science Foundation (OTKA, Grant No. 83886).

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c) herczku@atomki.hu

Establishing a dynamical equilibrium in electron transmission through insulating microcapillaries

A. R. Milosavljević[a], K. Schiessl[b], C. Lemell[b], M. Mátéfi-Tempfli[c], S. Mátéfi-Tempfli[c], B. P. Marinković[a] and J. Burgdörfer[b]

[a]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[b]*Inst. for Theoretical Physics, Vienna Univ. of Technology, Wiedner Hauptstr. 8-10, 1040 Vienna Austria*
[c]*Université Catholique de Louvain, Place Croix du Sud, 1, B-1348 Louvain-la-Neuve, Belgium*

We study the time dependence of electron transmission through microscopic (length 15 μm, diameter 270 nm) Al_2O_3 capillaries [1]. As in the case of ion transmission dynamical equilibrium is reached after some time [2]. Here, however, transmission sets in "immediately" (detection limit corresponds to about 50 nC deposition of charge) and reduces to its equilibrium value while for ions the charge-up time is required to build a charge patch in the entrance area of the capillary which deflects ions along the capillary axis.

We interpret this behavior based on a microscopic study of the process [3] in which the complete electron-insulator interactions sequence is taken into account. As electrons cannot change their initial charge state, charging of the surface can occur only if either the electron enters the target and is captured there (negative charge-up) or if interactions between the energetic primary electron and electrons in the valence band of the target lead to the emission of low-energy secondaries (positive charge-up). In the latter case, electrons are attracted to the surface rather than being deflected by Coulomb forces. This will lead on the one hand to a reduction of electron transmission as a function of time; on the other hand, however, (local) positive charging will enlarge the surface barrier and reduce the amount of low-energy electrons emitted. Eventually, a dynamical equilibrium will be established.

Indeed, this behavior is found in our experiments (see Fig. 1b) indicating a secondary-electron emission yield $\gamma > 1$ which is also corroborated by independent experimental data [4] and the large fraction of low-energy electrons exiting the capillary target (Fig. 1a).

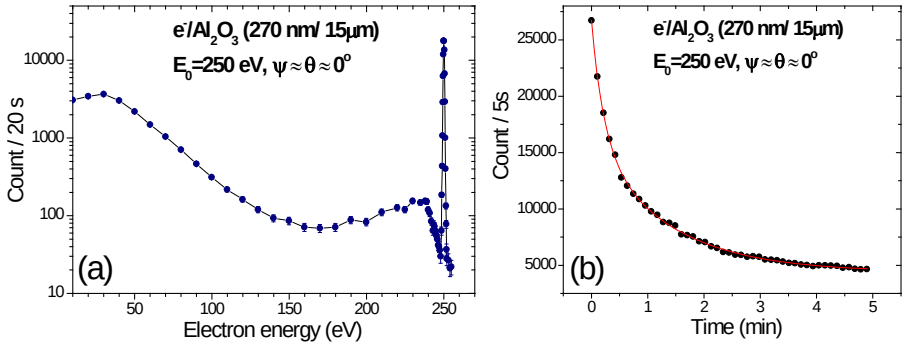

Fig.1. Electron transmission through an insulating Al_2O_3 capillary as a function of energy (a) and time (b). Secondary (low-energy) electron emission leads to local charge-up of the inner capillary wall reducing the transmission rate.

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Can positrons be guided by insulating capillaries?

R. D. DuBois[a] and K. Tökési[b]

[a]*Department of Physics, Missouri University of Science and Technology, Rolla, MO, USA*
[b]*Institute o f Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary*

During the past decade, a new phenomenon, namely "guiding" of charged particles through insulating capillaries, has been investigated using positive ions and electrons. The present study was initiated to investigate whether low-intensity positron beams can also be guided and, if so whether a tapered capillary might be used to reduce and improve the quality of low-energy positron beams.

This was done by modifying the positron apparatus at Missouri S&T which is normally used for differential ionization measurements. The modifications consisted of removing the target and scattered projectile spectrometer, installing a holder for several tapered capillaries that were fabricated at ATOMKI, Hungary, plus placing a position sensitive channelplate such that it could detect any positrons exiting from the capillaries. The holder could be moved horizontally and rotated vertically with respect to the incoming beam. Capillaries that were used had large input diameters (approximately 7 mm) and were tapered at approximately 8^o to small exit diameters ranging from 0.5 to 1.8 mm. A 6 mm diameter aperture was used to collimate the beam just before the capillary entrance.

Using sub-femtoamp beams of positrons and electron beams a factor of 10-50 more intense, possible guiding by three different tapered capillaries (2 glass and 1 teflon) was studied. For beam energies between 100 and 500 eV, the transmitted beam profiles and intensities were measured as functions of the capillary tilt angle (between 0 and 5 degrees). The transmitted intensity as a function of the total charge entering the capillary (up to 6 and 100 nCoul for positrons and electrons, respectively) was also measured. In addition, a search for any positronium that was produced during transit through the capillary was performed.

Our studies demonstrated that a portion of the entering beams were transmitted and that the emerging intensities followed the direction of the capillary and depended on the tilt angle. Both of these indicate guiding. However, we were unable to definitively rule out the possibility that the transmitted beams result from different input angles associated with our diffuse beams. Our measurements of the transmitted intensity as a function of charge entering the capillary were also inconclusive since no major increases in the transmitted intensity were observed. This could mean that insufficient charge was deposited or that charge patches were not able to form because the charging rate was too small with respect to the discharging rate. To investigate these aspects further, transmitted of low energy positive ion beams is currently being investigated. Additional details and results will be presented.

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Identification of the types of carbon nanotubes using donut effects

D. Borka[a] , V. Lukic[b], J. Timko[c] and V. Borka Jovanović[a]

[a]*Atomic Physics Laboratory (040), Vinča Institute of Nuclear Sciences, University of Belgrade, P. O. Box 522, 11001 Belgrade, Serbia*
[b]*Department of Bioengineering, University of Pennsylvania, Philadelphia, PA 19104, USA*
[c]*School of Physics, University of Sydney, NSW 2006, Australia*

We perform Monte Carlo computer simulations to determine the angular and spatial distributions of protons channeled through (6, 4), (8, 6), (11, 9) and (15, 10) single-walled carbon nanotubes of length 1 μm. The interaction between the protons and nanotube atoms is described by the Doyle-Turner interaction potential and the initial energy of the protons is varied from 10 MeV to 40 MeV. Angular and spatial distributions are calculated by solving the equations of motion for the proton in the transverse position plane inside the nanotubes [1]. We demonstrate that the trajectory of a proton through each nanotube is highly dependent on both the proton incident angle and the initial proton energy. As the proton incident angle approaches the critical angle for channeling, a ring-like structure develops in the angular distribution. This is known as the donut effect [2]. We show that the donut effect is very sensitive to the type of carbon nanotube and can be used to identify and characterize carbon nanotubes of different types.

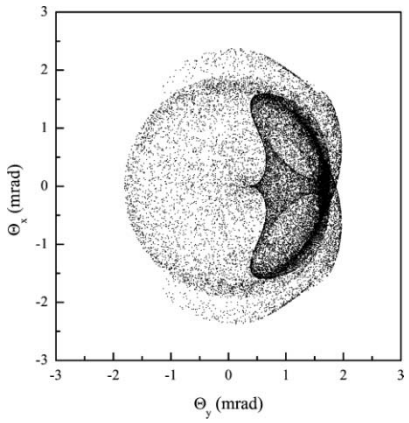

Fig.1. The angular distribution of channeled protons with the proton incident angle φ = 1.7 mrad in the (6, 4) SWCNT.

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Correlation between thermal induced structural and magnetic transformations in Si-rich $Fe_{73}Cu_1Si_{16}B_7Nb_3$ metal alloy

R. Brzozowski[a], M. E. Moneta[b]

[a]*Uniwersytet Łódzki, Katedra Fizyki Jądrowej, Pomorska 149, PL 90-236 Łódź, Poland*
[b]*Uniwersytet Łódzki, Katedra Fizyki Ciała Stałego, Pomorska 149, PL 90-236 Łódź, Poland*

X-ray diffraction (XRD), Mossbauer spectrometry (TMS), thermomagnetometry (TM) and scanning callorymetry (DSC) were used for characterization of amorphous $Fe_{73}Cu_1Si_{16}B_7Nb_3$ foil, the Si rich metal alloy, and the foils partly crystallized after annealing [1]. Fe(Si) and Fe(B) structures were identified [2,3] and characterized with the crystallization temperatures: 750K and 893K, activation energies 460kJ/mol and 580kJ/mol. The Curie temperatures for amorphous structure: 613K and for crystalline structures: 820K, 875K, 920K and 980K were determined.

A delay of the sample magnetization, determined by thermo-magnetometry (TM), with respect to structural crystallization, determined by scanning callorimetry (DSC), which was correlated with magnetic hyperfine field, determined by transmission Mossbauer spectroscopy (TMS), was found and analyzed, as it is shown in Fig(1).

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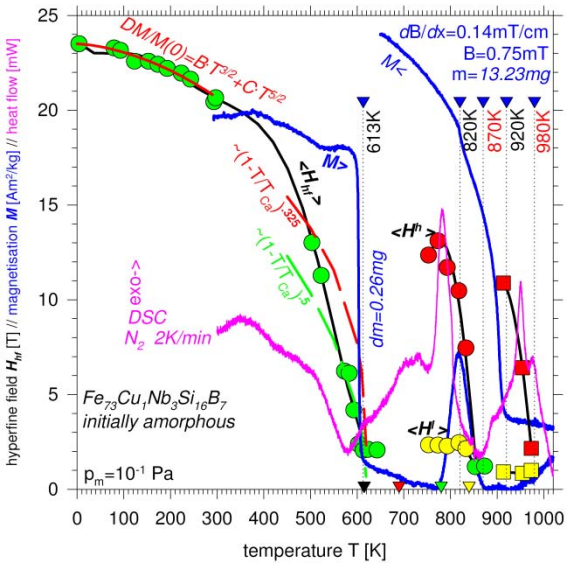

Fig.1. TMS hyperfine field H_{hf} (green, red and yellow symbols + black line), bulk magnetization M (blue line) and DSC scan (pink line) for $Fe_{73}Cu_1Si_{16}B_7Nb_3$ as functions of temperature T. The Curie points marked by dotted lines. Vacuum in the chamber $p_m=10^{-1}$Pa. Each measurement time t_m =12h. Low temperature magnetization: $\Delta M/M(0)=B\cdot T^{3/2}+C\cdot T^{5/2}$ with red line, the fitting parameters: $B\approx1.7\cdot10^{-5}K^{-3/2}$, $C\approx2.1\cdot10^{-8}K^{-5/2}$, $T_{Ca}\approx613$K. High temperature approximation with critical exponents: $\alpha=0.325$ - Heisenberg model (red dashes) and $\alpha=0.5$ - Weiss model (green dashes).

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Role of Ta replacing Nb in finemet alloy

A. Puszkarz[a], M. E. Moneta[b]

[a]*Politechnika Łódzka, Katedra Fizyki Molekularnej, Żeromskiego 116, PL 90-924 Łódź, Poland*
[b]*Uniwersytet Łódzki, Katedra Fizyki Ciała Stałego, Pomorska 149, PL 90-236 Łódź, Poland*

FeSiB finemets are known from 1988 as soft magnetic materials of high permeability (~10^5 at 1kHz), large magnetization (~1.2$T), low magnetostriction (~10^{-6}), low coercivity (~0.5A/m) and power loss (~38W/kg at 0.2T, 100kHz). The metal alloys, like $Fe_{73.5}Cu_1Si_{13.5}B_9Nb_3$ Finemet, consist primarily of amorphous-magnetic phase which, after appropriate thermal or mechanical treatment, are transformed into the phase in which iron-silicides and borides magnetic nano-crystals are embedded in an amorphous residual matrix. An important task is to keep size of the nano-crystals smaller than the exchange-correlation length.

So far many different modifications of the basic FeSiB composition were analyzed in search for better technical properties. In this work selected properties of Finemet[@] with Ta successively substituted for Nb, were analyzed. It can be expected that heavier, but belonging to the same Va group Ta would more than Nb retard nano-crystal growth due to larger atomic size and weaker diffusion [1,2].

Properties of Finemet[@] alloys $Fe_{73.5}Cu_1Si_{13.5}B_9Nb_{3-x}Ta_{x=0,1,2,3}$ with Nb successively replaced by Ta were studied experimentally. The as-prepared amorphous foils and these crystallized after conventional annealing were analyzed structurally and magnetically. X-ray diffraction (XRD), differential scanning calorimetry (DSC), transmission Mossbauer spectroscopy (TMS) and energy disperse X-rays (EDX) were used for analysis. XRD scans of annealed alloys show crystalline phases, corresponding to that for pure Finemet[@]. TMS spectra reveal typical hyperfine structure of annealed nano-crystalline phase embedded in amorphous reminder. EDX show good agreement between nominal and measured atomic content for all alloys.

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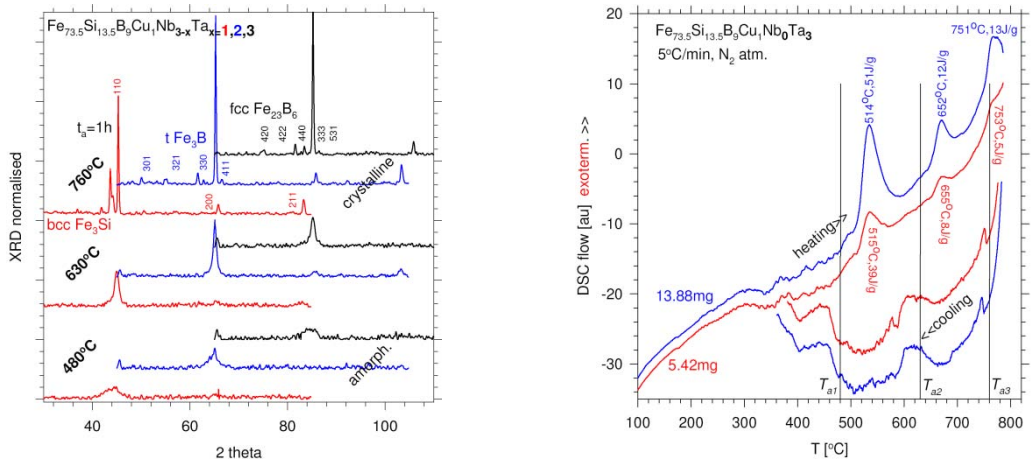

Fig.1. (colour online) Left: XRD angular scans of $Fe_{73.5}Cu_1Si_{13.5}B_9Nb_{3-x}Ta_{x=1,2,3}$ alloys annealed at 480, 630 and 760°C for time 1h [1,2]. Right: DSC scans at heating rate 5°C/min of the same alloys with identification of the onset points and specific enthalpies for the primary (peak 1), secondary (peak 2) and ternary (peak 3) crystallization, in dependence on content of Ta. Lines guide the eye.

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Depth selective PIXE for surface analysis with low energy heavy ions

B. Pawłowski[a], M. E. Moneta[a]

[a]*Uniwersytet Łódzki, Katedra Fizyki Ciała Stałego, Pomorska 149, PL 90-236 Łódź, Poland*

The interest in PIXE [1-2] is recently growing, since it slightly moved from basic research on characteristics of shell excitation, to application in biology, archeology and art. Also recently a particular attention is paid to external beam with a micro- and even nano-meter spot size for the applied research. For PIXE analysis usually MeV energy light particles are used, mainly protons from accelerators and cyclotrons, since *x*-ray emission cross-sections peak at these energies.

The advantage of low voltage accelerators, like Cockroft-Walton multiplier, working in the range from 30 to 400 kV, is that the ion penetration depth does not exceed a micrometer and the real surface composition *x*-ray analysis can be effectively performed. Moreover, the atomic shell excitation process does not critically depend on fluctuation of beam energy, beam intensity or vacuum condition. Disadvantage is much lower *x*-ray emission cross-section, for instance for p^+ in P: $\sigma_k \approx 65$ barn for E_p=200keV and 1600 barn for E_p=400keV, and roughly 10^3 times less for Cu. The cross section can be considerably enlarged by the use of heavy ions, which however cause sputtering, produce their own characteristic *x*-rays and this make analysis complicated due to large Coulomb interaction or molecular effects. On the other hand, shallow penetration depth predestinates heavy ions for analysis of thin films and subsurface regions.

A low energy heavy ions PIXE set-up was applied for search of trace elements in the subsurface regions. Analysis of elemental composition of standardized foils and thin films PVD evaporated on various substrates at LN_2 temperature was performed with the help of GUPIX codes, Fig.1a,b. Results for the k-shell x-ray emission cross-sections for selected elements were compared to results obtained with swift light ions.

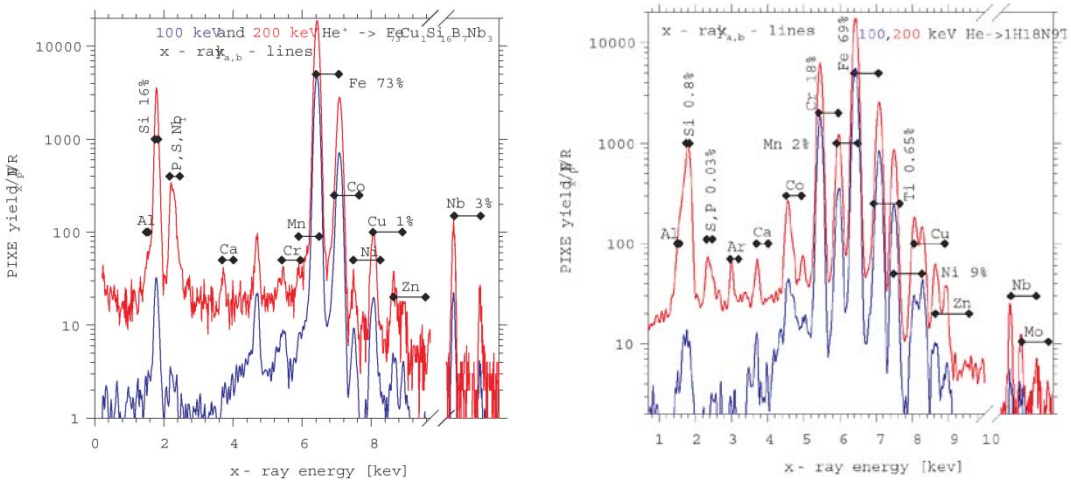

Fig.1. PIXE spectra generated by 100 keV He ions (projected range R=340nm) and by 200 keV He (R=580nm) in subsurface region of bulk $Fe_{72}Cu_1Si_{16}B_7Nb_3$ (a) and $Fe_{69}Cr_{18}Ni_9Mn_2Ti_{0.7}Si_{0.8}C_{0.1}P_{0.04}S_{0.03}$ (b). The nominal composition indicated in % and the trace elements printed in *italics*.
The spectra were measured with the Amptek *X*-123SDD spectrometer with resolution FWHM=120eV.

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Mössbauer distribution fitting by using global optimization approach

T. M. Gwizdałła, M. E. Moneta

Dept. of Solid State Physics, University of Łódź
Pomorska 149/153, 90-236 Łódź, Poland

The curve fitting issue is the problem, which is often studied by using the global optimization techniques. There is also many physical problems, especially those related to the analysis of experimental data, studied with the use of different optimization algorithms. Usually the methods of analytical optimization cannot be use since the computational effort is NP-complex. Among the existing solutions of such problems we can show e.g. the papers related to the structure determination on the basis of diffraction pattern [1] or the R-factor analysis for the LEED method [2]. There exist also several approaches when GO algorithms are used to reconstruct the structure of Mössbauer spectrum [3-6]. One should point out that all papers mentioned above deal with the specific, probably most popular in physical applications, form of global optimization – the genetic algorithm.

In our paper we present the comparison of two global optimization techniques – the genetic algorithm (GA) and the particle swarm optimization (PSO). We describe the choice of operators and their influence on the efficiency of calculations. We analyze also the size of the basin of attraction of the global minimum. This value is especially important because our algorithm is indeed the hybrid one. After the initial phase performed by using the GA or PSO method we exploit the solution using the local search algorithm, which is the form of the Hooke-Jeeves algorithm. We analyze the dynamics and efficiency of optimization for distributions containing up to four sextets.

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Study on the photo-induced oxygen reordering in $YBa_2Cu_3O_{6+x}$

M. M. Milic[a], N. Dj. Lazarov[a], D.A. Cucić[b]

[a]*Laboratory of Theoretical Physics, INN Vinča, University of Belgrade, P.O.Box 522, 11001 Belgrade, Serbia*
[b]*RCT Michael Pupin, Vojvode Zivojna Misica 6, 26000 Pancevo, Serbia*

Effect of the long term illumination of the $YBa_2Cu_3O_{6+x}$ with visible light or ultraviolet irradiation on its superconducting properties was studied in the frame of a simple theoretical model, which assumes that photodoping triggers rearrangement of oxygen monomers in the chain layers thus causing the enhancement of the average chain length, l_{av}. Since, according to the model of charge transfer mechanism, long CuO chains are better electronic hole donors than the short ones, increase of the average chain length induces additional holes transfer from chain layers to the superconducting CuO_2 planes which in turn leads to the increase of the superconducting transition temperature T_c. By the use of the expression for the chain length probability distribution and numerically calculated values for the average chain length in the non-excited system, we were able to estimate the doping p (number of holes per one Cu atom in the superconducting CuO_2 planes) and T_c enhancement due to photo-induced oxygen reordering. The theoretical results are compared with available experimental data.

Acknowledgements: This work is supported by the Ministry of Science and Technological Development of Republic of Serbia under project. No. 171027

Effect of illumination on the superconducting transition temperature T_c in $YBa_2Cu_3O_{6+x}$

N. Dj. Lazarov [a], M. M. Milic [a], V. M. Matic [a], D.A. Cucić[b]

[a]*Laboratory of Theoretical Physics, INN Vinča, University of Belgrade, P.O.Box 522, 11001 Belgrade, Serbia*[a]
[b]*RCT Michael Pupin, Vojvode Zivojna Misica 6, 26000 Pancevo, Serbia*

In the present study, we have employed two dimensional ASYNNNI model and the numerical Monte Carlo simulations to investigate the effect of visible light or ultraviolet radiation on the doping p of the superconducting CuO_2 planes, and consequently on the superconducting transition temperature T_c, in $YBa_2Cu_3O_{6+x}$ high-T_c superconductor. It was shown that, depending on the oxygen concentration, x, three regions of different critical temperature's T_c behavior can be distinguished. In the first region where $x<6.6$ the critical temperature increases rapidly with oxygen depletion, in the second region, $6.6<x<6.75$, the total T_c increase, δT_c, is almost independent of the oxygen content thus forming some kind of plateau, while in the third region, $6.75<x>7.00$, the T_c does not increase significantly. Such a theoretically obtained behavior of T_c is in general agreement with the experimentally established facts on the δT_c vs. x dependence.

2nd National Conference on Electronic, Atomic, Molecular and Photonic Physics

PLENARY LECTURES

Dynamics of dissociative electron attachment to small molecules

J. Fedor[a], O. May[a], D. Kubala[a], M. Allan[a]

[a]*Department of Chemistry, University of Fribourg, Chemin du Musée 9, 1700 Fribourg Switzerland*

Only few experimental techniques allow for tracking the motion of nuclei in molecular dynamics. They of course include time-resolved experiments with femtosecond lasers, that are nowadays relatively common. However, such experiments require very sophisticated (and expensive) laser equipment. The resonant scattering of slow electrons provides an alternative way to information about nuclear dynamics, via measuring cross sections for individual scattering channels and using isotopical substitutions in the studied molecules.

In this work we demonstrate, how measuring cross sections for the dissociative electron attachment channel unravels the dissociation dynamics of the transient negative ions. We present an experimental setup that combines the total ion collection and time-of-flight quantitative mass spectrometer, so that two independent values are obtained for each cross section [1, 2]. We concentrate on the DEA dynamics in small polyatomic molecules – C_2H_2 [1], C_4H_2[2] and HCN[3]. We show, how isotopically substituting hydrogens for deuterium changes the dissociation timescales and leads to shift in the competition between dissociation and electron autodetachment. The change of cross section in isotopically substituted species is indicative of the dissociation path. Since resonant electron scattering is a process that is difficult to describe theoretically, our measurements are also serve as a test for the accuracy of various theories

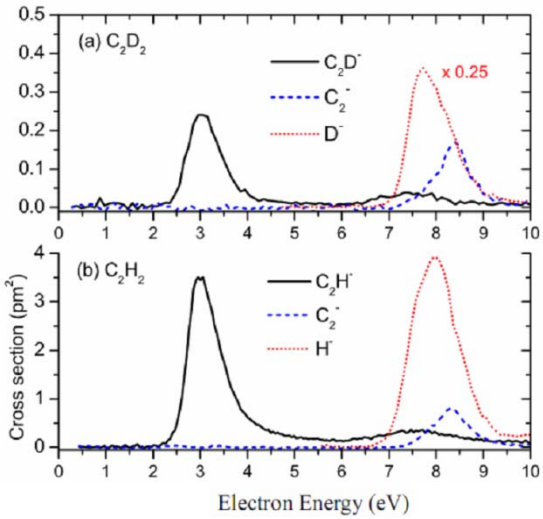

Fig.1. DEA cross sections for acetylene C_2H_2 and its deuterated analogue.

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Soft X-ray spectroscopy of molecules and biomolecules

C. Nicolas

SOLEIL Synchrotron, Saint-Aubin, France

Grazing incidence fast atom diffraction on different materials

N. Bundaleski[a], P. Soulisse[b], A. Momeni[b], H. Khemliche[b], P. Roncin[b]

[a]*CeFiTec, FCT, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal*
[b] *ISMO, CNRS, Univ. Paris-Sud, F-91405 Orsay cedex, France*

Fast atom diffraction at grazing incidence (GIFAD) discovered few years ago [1, 2] is a novel manifestation of quantum mechanics that has attracted quite some attention. It unambiguously demonstrates quantum scattering of atoms with energies in the range 0.1 – 2 keV along the channeling direction of ionic crystals at grazing incidence. The discovery was rather surprising due to the very short wavelength of such atoms (in the picometer range) with respect to the interatomic distances in solids. This paradox can be understood [1] assuming an efficient decoupling of the motion parallel and perpendicular to the surface, the latter having an associated wavelength in the Angstrom range for light projectiles. It was first assumed that the large band gap of ionic insulator is mandatory to prevent electronic excitations triggered by the fast parallel motion. These excitation being expected to introduce large decoherence leading to a destruction of the diffraction pattern. Latter on, diffraction was observed on semiconductors [3] and even metals [4,5], proving that the previous assumptions were wrong. This makes GIFAD a suitable technique for the surface analysis, for instance in a MBE environment. The intensity of the diffraction peaks is governed by the atom surface potential, i.e. the same interaction as in an AFM or in thermal helium diffraction. The analysis of the diffracted intensities therefore provides a highly accurate view of the surface topology. For instance, it was proposed [6] that the Li plane is shifted by some 0.053 angstroms with respect to the F plane at the surface of a LiF(001) crystal.

At variance, the analysis of the incoherent part of the signal provides direct information on the various sources of decoherence such as excitation of phonons or electrons. The latter can be identified by simultaneous energy loss measurements [4].

Experimental results of GIFAD on surfaces of insulators, semiconductors and metals will be presented and discussed. A particular attention will be paid to the various decoherence effects related to the atomic vibrations, electron excitations and the atomic beam properties.

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PROGRESS REPORTS

Theoretical study of the Jahn-Teller effect

M. Gruden-Pavlović[a], M. Zlatar[b] and C. Daul[b]

[a]*Faculty of Chemistry, University of Belgrade, Serbia*
[b]*Department of Chemistry, Faculty of Science, University of Fribourg, Switzerland*

Jahn-Teller (JT) type distortions include proper JT distortions of molecules in a degenerate electronic state, Pseudo JT (PJT) distortions in non-degenerate electronic states, and Renner-Teller (RT) distortions in a linear system. Any structural distortion of a polyatomic system is of the JT, PJT, or RT origin. Many interesting problems in modern chemistry and solid-state physics have been successfully explained within the framework of the JT effect.

Density Functional Theory (DFT) is today the most common theoretical method in quantum chemistry, and it can be successfully applied for a detailed analysis of the JT effect. The analysis of the structural distortion from the high symmetry (HS) nuclear arrangements of JT active molecules presents a challenge because of the superposition of the effects produced by different normal modes. In order to tackle this problem, we have recently proposed to express the JT distortion as a linear combination of all totally symmetric normal modes in the low symmetry (LS) minimum energy conformation, which allows calculating the Intrinsic Distortion Path (IDP), exactly from the high symmetry point to the low symmetry configuration. The aim of the present work was to calculate reliable values of the JT parameters for different JT active molecules, and to try clarifying which and how the different totally symmetric normal modes of the LS structure contribute to the JT distortion. Conceptually simple model gives the direct insight into the one of the essential problems in the physical chemistry-coupling between the electron distribution and the motion of the nuclei.

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Theoretical investigation of vibronic and spin–orbit effects in the ground $X\ ^2\Pi_u$ electronic state of dicyanoacetylene cation

R. Ranković, S. Jerosimić and M. Perić

Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12, P.O. Box 47, PAC 105305, 11158 Belgrade, Serbia

The aim of the present study is to elucidate some controversial details in the observed NC_4N^+ spectra, by means of *ab initio* calculations. The structure of the ground electronic state, $X\ ^2\Pi_u$, of NC_4N^+ was investigated by the density functional (B3LYP) and multi-reference configuration interaction (CASSCF-MRCI) methods. The bending vibrational frequencies ω_{T1} = 558 cm^{-1}, ω_{T2} = 266 cm^{-1}, ω_{C1} = 459 cm^{-1}, and ω_{C2} = 113 cm^{-1} were obtained. The spin–orbit coupling constant was calculated using the state-average CASSCF wave functions in the framework of the MRCI method, and the value of A_{SO} = −44.29 cm^{-1} was determined. The data for the bending frequencies and Renner parameters were employed for handling the combined effect of the vibronic and spin–orbit coupling, according to a recently developed model [1,2].

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Excitation of molecules by low-energy electrons

M. M. Ristić

Faculty of Physical Chemistry, University of Belgrade, P.O. Box 137, 11000 Belgrade, Serbia
Faculty of Physics, University of Belgrade, Studentski trg 12, 11000 Belgrade, Serbia

Excitation of the H_2 and CO molecules with low energy electrons has been investigated by use of a crossed beam double trochoidal electron spectrometer in pulsed mode of operation. Contributions of forward and backward scattered electrons have been separated by electron beam modulation and time-of-flight detection of scattered electrons [1], [2]. The ratio of forward-to-backward signal is equal to the ratio of differential cross sections at 0 and 180 degrees.

The forward and backward scattered electrons from the $^2\Sigma_u^+$ shape resonance in the v=0→1 vibrational excitation channel of the H_2 molecule have been analyzed. Impact electron energies have been varied from 1 to 5 eV. The same type of experiment has been performed for analyzing electrons in resonant excitation of ground vibrational level of the $a^3\Pi$ valence state of CO, with impact electron energies from threshold to 9.7 eV.

In both cases, the appropriate normalization procedure has been applied in order to obtain the absolute differential cross section values at 0 and 180 degrees. Comparison with available experimental measurements [2]-[6] and theoretical predictions [7], [8] has been made. In this way the differential cross section measurements are completed in the full angular range from 0 to 180 degrees. Obtained angular distributions can be used for exact modeling of electron movement through the atmospheres of H_2 and CO, but also for precise determination of integral cross sections at given electron energies.

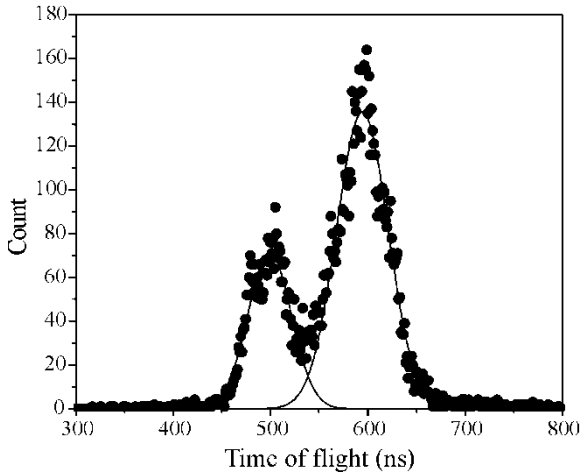

Fig.1. Time-of-flight spectrum of electrons scattered at 0^o and 180^o from the $v = 0$ level excitation of the $a^3\Pi$ state of CO at an incident energy of 7 eV

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Absolute cross sections for electron excitation of silver

S. D. Tošić[a], V. Pejčev[b], D. Šević[a] and B. P. Marinković[a]

[a] *Laboratory for Atomic Collision Processes, Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[b] *Faculty of Natural Sciences, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia*

The differential cross sections (DCSs) are widely used experimental tools in the study of electron interactions with different atoms. In electron-atom scattering processes, DCS is used to describe the strength of interactions among atomic particles, i.e. to relate the impact parameter to the scattering angle of a particle that has experienced a collision with the force field of another particle. Generally, this observable gives the probability of specific interaction at certain electron energy and scattering angle. To determine absolute DCS it is necessary to know absolute atom target density and its spatial distribution, energy and angular distribution of electron beam and its current density, as well as effective scattering volume [1] and response function of detection system.

In the Laboratory for Atomic Collision Processes of the Institute of Physics in Belgrade, we undertook a series of electron spectroscopic measurements to study electron collision with metal atoms. The experimental method used to determine differential cross section (DCS) is based on crossed beam technique in the electron spectrometer ESMA, described in details elsewhere [2]. Monoenergetic electron beam was obtained by means of hemispherical selector and it is focused by cylindrical electrostatic lenses. Electron beam of energies from 10 to 100 eV was perpendicularly crossed by effusive atomic beam formed by heating oven crucible containing metal atoms. Elastically and inelastically scattered electrons were energy analyzed by the selector, and were detected by a single-channel electron multiplier. Absolute values for the resonance states are obtained by normalization of relative differential cross sections to the optical oscillator strengths [3], while the absolute values for the elastic scattering and excitations other than resonance are obtained from the intensity ratios at particular scattering angle(s).

Here we present results of our experimental investigations of the electron excitation of the ground $4d^{10}5s$ state of silver. DCSs for excitation of the combined resonant $4d^{10}5p$ state (two fine-structure levels with total angular momentum J = 1/2 and 3/2 which cannot be distinguished in the present experiment) were measured at electron-impact energies (E_0) of 10, 20, 40, 60, 80 and 100 eV and for a range of scattering angles (θ) from 1^o up to 150^o. Absolute DCSs were obtained through the procedure of normalization which was described elsewhere [4]. Other details will be presented at the conference.

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Coherent effects in laser driven rubidium vapor

M. Radonjić, A. Krmpot, S. Ćuk, S. Nikolić and B.M. Jelenković

Institute of Physics, University of Belgrade, Pregervica 118, 11080 Belgrade, Serbia

Some of recent results concerning Electromagnetically Induced Transparency (EIT) resonances in laser driven *D1* line transition $F_g = 2 \rightarrow F_e = 1$ in rubidium vapor in Hanle configuration [1,2] will be presented. It will be discussed how laser intensity and beam profile (Gaussian or Π-shaped) influence the shapes of Hanle EIT resonances. Our analysis of the Hanle EIT resonances obtained in the selected segments of the Gaussian or Π-shaped laser beam cross section reveals the details of the evolution of atomic system traversing the laser field of a given profile. Significant differences in the Hanle EIT line-shapes are observed depending on whether the central or outer parts of the laser beam are detected in case of both used beam profiles. The line narrowing and two counter-sign peaks occur at *outer*, less intense parts of the *Gaussian beam* due to the interference of the laser light and coherently prepared atoms coming from the central part of the beam [1]. In contrast to the Gaussian beam, the narrowing of the Hanle EIT resonances and two counter-sign peaks occur in the *central* parts of the *Π-shaped beam* cross section [2]. These counter-sign peaks are not of coherent nature, but appear due to optical pumping to the uncoupled $F_g = 1$ level while the resonance narrowing is attributed to the time of flight. Our studies indicate the importance of considering real radial laser beam profile for proper modeling and understanding of coherent effects in alkali metal vapors.

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Numerical modelling of buffer gas positron traps

S. Marjanović[a], M. Šuvakov[a] and Z. Lj. Petrović[a]

[a]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

Buffer gas positron traps are the prime tool for study of antimatter-matter interaction. They proved to be the source of data for binary collisions that made almost complete sets available for Ar, N_2, H_2 and recently H_2O. In return, we were able to use that data in our dedicated Monte Carlo simulation scheme to model the operation of such traps in order to better understand the processes occurring inside. In such a model, we are free to change the composition and pressure of buffer gas in different stages of the trap, configuration of the electric and magnetic field and operation time, while monitoring loss processes and evolution of particle energy and spatial distribution. Thus we are able to optimize the parameters of the trap to increase its efficiency in respect to number of trapped particles, energy resolution, beam width and time of operation required for the particles to thermalize.

We will offer examples of trap configurations currently in use in several laboratories around the world and show the simulation results containing the temporal evolution of amount of particles lost to different events such as positronium formation, annihilation, escaping particles and losses to walls. In addition we follow the monoenergetic initial energy distribution into a broad swarm like distribution characteristic of later times.

Finally, we propose a novel trap scheme, based on previous calculations, with a buffer gas mixture containing predominantly CF_4, with a higher than usual pressure inside the trap.This design uses potentials, deliberately selected to avoid the process of positronium formation. Such a design demonstrates a significantly improved performance of the trap in both thermalization times and width of the beam, and leads to a several times larger total number of trapped particles.

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Monte Carlo modeling of Townsend discharges in hydrogen

V. Stojanović, Z. Petrović and Ž. Nikitović

Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

DC high E/N swarm experiment (self sustained discharge operating in Townsend regime of volt-current characteristics) may be modelled directly and exactly as it does not require self consistent calculation of the electric field. The Monte Carlo simulation could be selected as a best suited technique that may include complexity at the level of representation of collisional events being most important in swarm concept. Boundary conditions for swarm particles, introduced by metallic anode and cathode are simply added by knowing angular and energy distributions of the reflected particles.

In this paper we show how Monte Carlo technique developed for swarm studies may be applied to model some real discharges or to provide data for realistic plasma models. In all cases discussed here the Monte Carlo technique without self consistent field is driven to a much greater level of complexity than usually found in swarm studies.

Monte Carlo modeling results of electrons and heavy particles induced spatially resolved emission intensity and the Doppler profile of Hα line in pure H_2 discharge are presented. We used revised simple models of heavy particle collisions in hydrogen [1] appropriate for low pressure high electric field strengths. Our results, based on collision model that supports atom and ion excitations being the source of fast excited H atoms moving forward and away from the cathode, are in agreement with experimental data[2]. As one would expect the greatest contribution comes from the fast H atoms.

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On the propagation of positive streamers in N_2:O_2 mixtures

G. Wormeester[a], S. Nijdam[b], S. Dujko[a,c] and U. Ebert[a,b]

[a]*Centrum Wiskunde & Informatica, PO Box 94079, 1090 GB Amsterdam, Netherlands*
[b]*Department of Applied Physics, Eindhoven University of Technology, PO Box 513, 5600 MB, Eindhoven, Netherlands*
[c]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080, Belgrade, Serbia*

Streamers are thin channels of ionized gas that occur in nature (lightning and sprites) and have applications in industry (gas cleaning, lighting). We distinguish between positive and negative streamers, where positive streamers propagate against the electron drift velocity and require a source of free electrons in front of the streamer head. Experimental results have shown a remarkable robustness of positive streamers against changes in gas composition [1]. Using numerical simulations, we have studied the effect of microscopic properties, such as the source of free electrons and transport data, on the macroscopic streamer properties such as velocities and diameters for streamers in N_2:O_2 mixtures at standard temperature and pressure [2].

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POSTER CONTRIBUTIONS

An *ab initio* calculation of the vibronic energy levels in the $X\ ^2\Pi$ electronic state of C_2Sb

M. Milovanović, S. Jerosimić

Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12, P.O. Box 47, PAK 105305, 11158 Belgrade, Serbia

The results of an *ab initio* calculation of the vibronic energy levels in the ground $X\ ^2\Pi$ electronic state of C_2Sb are reported. This work is motivated by the recent theoretical studies of C_2P [1] and C_2As [2,3] carried out by our group; our results strongly supported the analysis of experimental data by Clouthier's group [4] and offered reliable predictions for experimental searches for heretofore unobserved electronic states. These species are interesting from the astrophysical/astrochemical point of view. As far as we know, there is no reported experimental data on this molecule.

The vertical electronic spectrum, excitation energies of low-lying doublet states, and spin-orbit constant for the ground state are computed by means of the state-average complete active space self-consistent field (CASSCF) [5] and multi-reference configuration interaction approach (MRCI) [6] incorporated in MOLPRO 2006.1 program package [7]. Geometry optimization, harmonic frequencies and bending potential curves of the ground state are calculated using the B3LYP functional in the aug-cc-pVTZ (C), aug-cc-pVTZ-PP (Sb) basis sets [8].

The potential energy curve for the ground $X\ ^2\Pi$ ($1^2\Pi$) state as a function of the bending coordinate ρ is computed in the range between $\rho = 0$ and $\rho = 40$ deg. The computations have been performed at the equilibrium geometry of the ground state, i.e at the bond-lengths kept fixed at the values of r(C-C) = 1.2838 Å, r(C-Sb) = 1.9437 Å (B3LYP) in the C_S point group.

The handling of the Renner-Teller effect has been carried out using the variational *ab initio* approach described in detail elsewhere [9]. We hope this investigation will be of great importance for future experimental investigations.

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Ab initio study of the non-adiabatic coupling between X^1A' and $2^1A'$ states of D_3^+ ion

Lj. Stojanović[a]

[a]*Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12, P.O. Box 47,PAC105305, 11158 Belgrade, Serbia*

The present study is concerned with diabatization of the ground (X^1A') and excited ($2^1A'$) states of D_3^+ ion and presents the first step towards description of the vibrational transitions between them in the region of their strong non-adiabatic coupling [1]. An extensive computation of the three-dimensional potential energy surfaces (PESs) is performed by means of the state-average complete active space self-consistent field with subsequent multireference configuration interaction approach (Fig.1.) [2]. The geometry of the localized conical intersection is optimized. Non-adiabatic coupling matrix elements (NACMEs) are computed within the examined region of the nuclear degrees of freedom. The form of the PESs and NACMEs has been discussed in terms of molecular structure. The states experience strong non-adiabatic coupling in the vicinity of the crossing seam. An *ab initio* quasi-diabatization of potential energy surfaces is carried out and residual non-adiabatic couplings are calculated [1], [3].

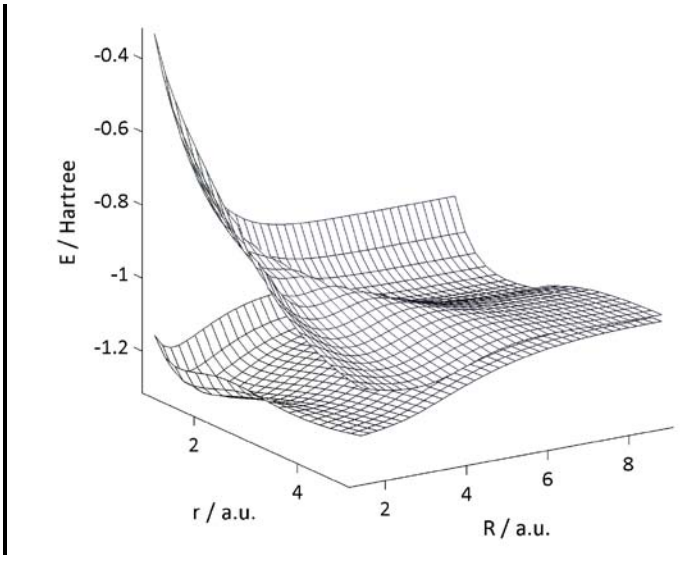

Fig.1. *Ab initio* adiabatic potential energy surfaces of X^1A' and $2^1A'$.

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Photon structure

N. V. Delić[a], B. Markoski[b], J. P. Šetrajčić[a], S. Armaković[a] and I. J. Šetrajčić[a]

[a]*University of Novi Sad, Technical Faculty Mihajlo Pupin Zrenjanin, Serbia*
[b]*University of Novi Sad, Department of Physics, Faculty of Sciences, Serbia*

Photon Hamiltonian which is given by (1), can be expressed by means of spin operators in the following form:

$$\hat{H} = \frac{2c}{\hbar}\left(\hat{S}_x\ \hat{p}_x + \hat{S}_y\ \hat{p}_y + \hat{S}_z\ \hat{p}_z\right) \tag{1}$$

The obtained form of photon Hamiltonian, which includes the operators of translation moment $\hat{\vec{P}}$ and spin $\hat{\vec{S}}$ suggest that a free photon has wealthy internal dynamics that consists of mutual action of its translation and spin characteristics. This "internal life" will be examined further in the paper[1].

In connection with this fact is the hypothesis that the photon is a bound state of neutrino and antineutrino. This hypothesis has been sent to CEWQO Symposium 2010 [2]. The hypothesis that the photon bound states of the neutrino and antineutrino has resulted in the first place that there are three types of photons, due to the fact that there are three types of neutrinos: electron, muon and tau neutrino [3]. The present viewpoint in science is that the photons differ in their energies, and taking into account the fact of equivalence of matter and energy, the different types of energy we can join to the different types of material photon.

$$\gamma_e = (\nu_e + \overline{\nu}_e) = \nu_e\overline{\nu}_e \tag{2}$$

$$\gamma_\mu = (\nu_\mu + \overline{\nu}_\mu) = \nu_\mu\overline{\nu}_\mu \tag{3}$$

$$\gamma_\tau = (\nu_\tau + \overline{\nu}_\tau) = \nu_\tau\overline{\nu}_\tau \tag{4}$$

It is important to note that the operation + means of bound states, which may not be valid energy conservation law (comes to the transfer of energy into information and vice versa).

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Confined hydrogen atom in the stationary electric field

Lj. Stevanović[a], V. Pavlović[a]

[a]*Department of Physics, Faculty of Sciences and Mathematics, University of Niš, Višegradska 33, 18000 Niš, Serbia*

The effect of the stationary electric field on hydrogen atom, confined by spherical box with impenetrable walls [1]-[3], is the subject of this work. Potential acting on the electron resembles double well structure, as it is shown on the figure. One of the wells is formed by Coulomb potential. The other well is formed by electric field potential and the wall of the infinite spherical well. Since the barrier, separating the wells is of finite height and width, the tunneling and corresponding resonant splitting between the lower levels take place. The variation of the energy level separations with radius of the confining sphere R_0, with emphasize on the values when simultaneous degeneracy between the pairs of confined hydrogen atom levels holds [4], and electric field strength, is investigated. The Schrödinger equation for the electron, moving in the combination of confining and electric field potentials, is solved by discretization method and with imposed Dirichlet boundary condition [5]-[7].

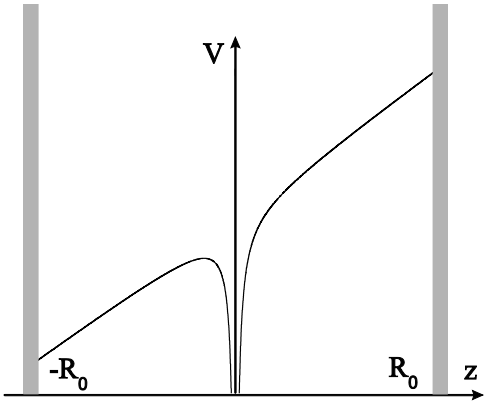

Fig.1. The form of the potential, composed from confining and electric field potentials, in the $\theta = 0$ direction

Acknowledgments: The financial support from the Ministry of Education and Science of Republic of Serbia is acknowledged.

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Properties of the F center based on the model of confined atomic system

Lj. Stevanović [a], V. Pavlović [a] , M. Rančić [a]

[a]*Department of Physics, Faculty of Sciences and Mathematics, University of Niš, Višegradska 33, 18000 Niš, Serbia*

Electron trapped by anionic vacancy in alkali halide crystal is the system on the borderline between atomic and solid state physics. This type of the lattice point defects, known as F center, absorbs and emits light like an atom. Although the close relationship between the free atom or ion and F center exists, there is fundamental difference regarding their optical properties [1]. This fact allows to treat the color center as an electron confined in nanometer sized cavity of a determined shape [2]. Our work is based on the model described in [3]: inside the cavity, electron is confined by spherical well of the depth V_0 and width r_0, and outside the cavity, electron is confined by Coulomb potential reflecting the polarisability of the crystal.

Within the proposed model of the hydrogen atom, confined by this specific potential, radial wave functions of the F center are given in terms of spherical Bessel function [4] and confluent hypergeometric function *U* [5]. Imposing the matching condition on logarithmic derivative of the wave function, the energies of the lowest states for some values of orbital quantum number, are obtained. The changes in energy and oscillator strength for the $1s \rightarrow 2p$ dipole transition are studied with variations in the parameters of the confining potential.

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Differential cross sections for Bremsstrahlung and pair production and for predicting Terrestrial Gamma – ray flashes

C. Köhn[a] and U. Ebert[a,b]

[a]*Centrum Wiskunde & Informatica (CWI), PO Box 94097, 1090 GB Amsterdam, The Netherlands*
[b]*Department of Applied Physics, Eindhoven University of Technology, The Netherlands*

The calculation of X-ray and gamma-ray emissions from fast electrons in air requires appropriate differential cross-sections for the Bremsstrahlung generated when an electron collides with a molecule. We reviewed the literature, performed the necessary integrations and will present the required effective parameters at the conference. Energy and angular distributions of photons are presented relative to energy and direction of the incident electron after the angles determining the direction of the outgoing electron have been integrated out.

We also provide cross sections for the production of electron positron pairs. For one particular type of pair production the cross section formulas show a so-called cross symmetry to the cross section for Bremsstrahlung so that Bremsstrahlung results can be taken over. Furthermore we have found cross sections for other processes creating positrons; however, these processes seem less likely.

Elastic electron scattering by bismuth

B. P. Marinković[a], V. Pejčev[a,b], B. Predojević[c] and D. Šević[a]

[a]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[b]*Faculty of Sciences, University of Kragujevac, R. Domanojevica 12, Serbia*
[c]*Faculty of Sciences, University of Banja Luka, Republic of Srpska, BiH*

Bismuth belongs to the sixth row and 15th group of Periodic Table of Elements, its atomic number is 83 and weight 208.980. The electronic configuration is [Xe] $4f^{14}$ $5d^{10}$ $6s^2$ $6p^3$.with the ground state of $^4S_{3/2}$ symmetry. We have measured the differential cross sections (DCS) for elastic electron scattering by bismuth at impact energies of 10, 20, 40, 60, 80 and 100 eV and scattering angles up to 150°. Electron spectrometer and experimental procedure had been described elsewhere [1,2].

Unpolarised beam of bismuth vapour (Bi and Bi_2) was perpendicularly crossed by unpolarised beam of electrons and elastically scattered electrons were detected with the angular resolution of 1.5°±0.2°. Williams *et al* (1975) had also measured elastic DCS but with lower angular resolution (2.5°±0.8°) and only at 40 eV impact energy [3]. Established absolute values for elastic DCSs could serve as a reference for normalization of the other measurements of elastic e/Bi scattering where the polarization of electron beam is determined after the scattering event [4]. Scilicet, polarisation effects can arise due to spin-orbit interactions with nucleus (Mott scattering) or due to fine-structure effect (interactions of electron-electron, exchange interaction, outer shell). Contrary to the case of lead which ground state configuration is of ($6s^26p^2$) ^3P_o symmetry and where both mechanisms are possible, in the case of bismuth, which ground state is with the zero total angular momentum so that the atomic orientation is not possible, the dominant process of obtaining polarized beam of scattered electrons is due to Mott scattering.

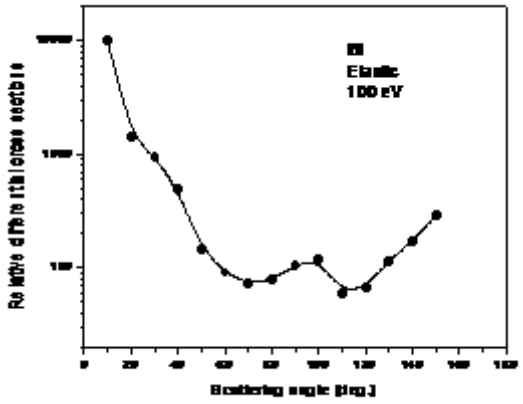

Fig.1. Relative differential cross sections for elastic electron scattering by bismuth

Acknowledgments: This work has been done within the projects MES RS OI 171020 and COST Action MP1002 "Nano-scale insights in ion beam cancer therapy (Nano-IBCT). We acknowledge the contribution of late Prof. D. M. Filipović.

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High resolution electron spectrometer OHRHA

J. J. Jureta, A. R. Milosavljević and B. P. Marinković

Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

New electron spectrometer OHRHA, **O**micron **H**igh **R**esolution **H**emispherical **A**nalyser, has been assembled for the first time in the Laboratory for Atomic Collision Processes at the Institute of Physics Belgrade. Beside other 3 electron spectrometers in the same Laboratory [1] all designed for studies of specific processes in electron collisions with atoms, molecules and metal vapours at low impact energy, the OHRHA spectrometer is designated for study processes at high electron impact energy.

The spectrometer OHRHA consists of high energy electron gun, high resolution hemispherical analyser, hypodermic needle as a source of effusive beam of target gas and a Faraday cup as a collector of electron beam. The electron gun is designed by Omicron Vakuumphysik Gmbh for electron impact energies from 10 eV to 1.5 keV (type EKF1000). In the first measurements its position is fixed at 90° in respect to gas beam and analyser (Fig 1). In the feature it will be mounted on the turn table that allows rotation around atomic beam axis. Hemispherical energy analyzer (EA 125 HR, Omicron) has a mean radius of 125 mm and variable entrance/exit slits of multi-element zoom lens. It is equipped with 7 channeltrons for electron detection. Ultimate projected energy resolution is of the order of 10 meV depending on the type of experiment. The vacuum chamber is home made and is pumped by the 3 turbo molecular pumps.

Fig.1. Top view of electron spectrometer OHRHA

The system has been tested for 500 and 800 eV electron impact energies scattered by argon atom. Spectra has been recorded and compared with other from the literature [2,3].

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Fast *in-vacuo* photon shutter for synchrotron radiation quadrupole ion trap tandem mass spectrometry

A. R. Milosavljević[a], C. Nicolas[b], J.-F. Gil[b], F. Canon[b], M. Réfrégiers[b], L. Nahon[b] and A. Giuliani[b,c]

[a]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[b]*Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, BP 48, 91192 Gif-sur-Yvette, France*
[c]*Cepia, Institut National de la Recherche Agronomique (INRA), BP 71627, 44316 Nantes Cedex 3,*

A special beam shutter has been designed as a part of the novel experimental setup for tandem mass spectrometry and ion spectroscopy of electrosprayed ions in a linear quadrupole ion trap using VUV and soft X-ray synchrotron radiation [1]. The irradiation of trapped precursor ions has been performed by coupling a commercial linear quadrupole ion trap ("Thermo scientific LTQ XL"), equipped with the electrospray ion source (ESI), to both VUV DESIRS beamline [2] and soft X-ray PLEIADES beamline [3] at the SOLEIL synchrotron radiation facility. The synchrotron beam is introduced into the trap through the back lens of the spectrometer.

The role of the mechanical shutter in the present experiment is to provide photon irradiation of the ions in the trap, starting at a desired moment and during well defined period of time. The most important conditions it has to fulfill are: the fast cut-off (on) of the photon beam (~ 1 ms), so well defined time of irradiation; fast response (~ 10 ms); robust design and stable, reproducible work during non-stop beam time period, under high vacuum conditions (10^{-7} mbar).

The design (Fig. 1) is based on the "KUHNKE" rotational electro motor which provides fast and reproducible work and 100% duty cycle. In order to preserve the fast rotation (thus, the fast beam on/off), a light pure aluminum hollow cylindrical shutter with two perpendicular holes has been fixed directly to the solid shaft of the electro motor. The construction with a shutter directly attached to the electro motor avoids a need for a special rotary motion vacuum feedthrough, which can increase the response and cut-off time. In order to avoid overheating, the body of the electro motor has been tightly attached to a special massive heat sink made of the oxygen free cupper.

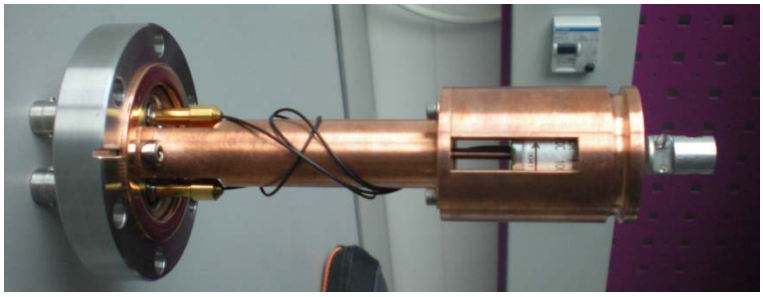

Fig.1. The photo of the mechanical photon shutter attached to the cupper heat sink and a vacuum flange.

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Analysis of cyanobacterial Cr-Phycoerithrin by laser based techniques

M. Terzić[a,c] M. S. Rabasović [a], D. Šević[a], A. Delneri[b], M.Franko[b] and B. P. Marinković[a]

[a]*Institute of Physics, University of Belgrade, P.O. BOX 68, Serbia*
[b]*Laboratory for Environmental Research, University of Nova Gorica, Slovenia*
[c]*Faculty of Science, University of Novi Sad, Serbia*

Phycoerythrin (PE) isolated from cyanobacteria, is an attractive fluorescent dye because it has a broad and high absorption of light over a wide range of the visible spectrum. The PE was among the first molecules to be observed at the single-molecule level using laser induced fluorescence [1]. PE fluoresces in a spectral region that is distinct from the region of emission of the simple organic dyes commonly used as fluorescent indicators. Therefore, PE is commonly used for fluorescent immunolabeling, particularly in applications involving fluorescent-activated cell sorting. Cr-Phycoerythrin (Cr-PE) is small phycobiliprotein (40-kDA) isolated from a proprietary cyanobacterium.

This work is focused on application of a high-sensitivity method of laser induced fluorescence [2] and thermal lens spectroscopy [3] for the analysis of Cr-PE. In the excitation wavelength range (340-470 nm) fluorescent spectra exhibit a pronounced maximum at 575 nm. Another maximum, at about 600 nm can be also observed. Beside this, the third emission maximum appears at about 519 nm.

The obtained results are used to verify the technical parameters of the used thermal lens technique, which is complementary to spectrofluorimetry and subject to lower sensitivity in case of high fluorescence quantum yields and photolability of measured compounds.

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The influence of radial laser beam profile on handle dark state evolution

S. N. Nikolić, M. Radonjić, S. M. Ćuk, Z. D. Grujić, A. J. Krmpot, B. M. Jelenković

Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
krmpot@ipb.ac.rs

In this paper we investigated the influence of two different laser beam profiles, the Gaussian and the Π-shaped profile, on the Hanle electromagnetically induced transparency (EIT) resonance lineshapes. The change of the shape of the Hanle EIT resonances obtained at different radial distances from the laser beam center directly reflects the evolution of the moving atomic system during the interaction with resonant laser light of constant intensity (Π-laser beam) and variable intensity (Gaussian laser beam). This work was motivated by the fact that the influence of different laser beam profiles on the shape of the Hanle EIT resonances is not thoroughly investigated and that the physical processes during the interaction of atoms with resonant laser light while atom is passing through the laser beam are not explained well enough. The influence of radial intensity distribution of the laser beam on coherent effects was previously studied in [1, 2]. Studies were done in the vacuum Rb gas cell with the laser resonant to the open $F_g=2 \rightarrow F_e=1$ transition at D1 line in ^{87}Rb. Hanle EIT resonances were measured and calculated for two different beam profiles of the same beam diameter.

Significant differences in the Hanle lineshapes are observed depending on whether the central or outer parts of the laser beam are detected. The line narrowing and two counter-sign peaks occur at outer, less intense parts of the Gaussian laser beam, while in the case of a Π-shaped profile these effects were observed in central segments of the beam. Excitation in the wings of the Gaussian beam profile produces narrower lines compared to the central part of the beam due to repeated interaction of atom and photons. Atoms are first coherently prepared in the intense central region of Gaussian beam, and afterwards "probed" in the laser wings [3]. On the other hand, atoms entering Π-shaped beam become coherently prepared into the stationary dark state. Average time spent by atom inside the beam increases with approaching the beam center, so that resonance narrowing in central segments is due to the time of flight.

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Air-ion counter and mobility spectrometer

P. Kolarž[a] and B. Miljković[b]

[a]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080, Belgrade, Serbia*
[b]*Merni instrumenti D.O.O., Ljube Stojanovica 38, 11000, Belgrade, Serbia*

Mono-electrode air-ion counter and mobility spectrometer based on the Gerdien aspirated condenser principle (Gerdien, 1905) has been developed. Instrument is intended for indoor and outdoor measurements of both air ion polarities (Fig.1).

Measuring small currents (~10^{-14} A) generated by the air-ions in outdoor conditions is demanding and causes many problems related to change of temperature, high humidity and wind. Also, measuring of both ion polarities with mono electrode detector require alternate changes of the polarizing voltage that causes series of noise sources which are corrupting zero conductivity determination. This, and problems like influence of temperature changes on the amplifier and zero drift are compensated using automatic zeroing (Kolarž et al., 2005).

Current leakage on electrodes and amplifying unit, caused by high humidity is prevented by measuring electrode rubin ball bearing system and also by heating the electronics and ball bearers. Influence of wind on air-flow through the interelctrode system is partially compensated by keeping the RPM of the fan constant. Size i.e., mobility, categorisation of air ions is done by programmable controlled cascade polarization voltage change by 0.5 V from zero up to 200 V. Dependence of ion mobility on particle mass diameter is calculated using the algorithm given by Tammet, 1995.

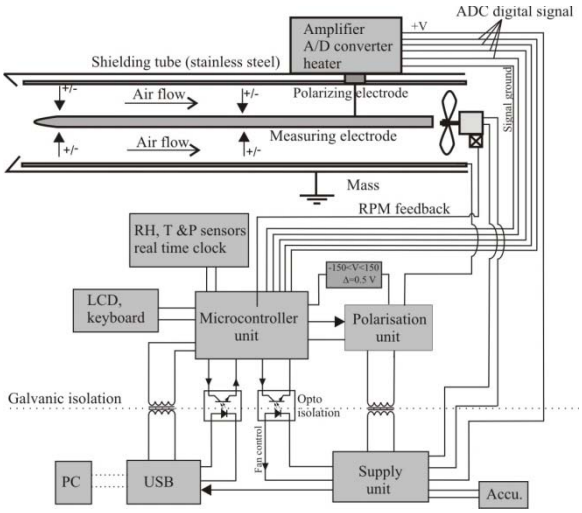

Fig.1. Block diagram of the Mono-electrode air-ion counter and mobility spectrometer.

Acknowledgments: *Ministry of Education and Science of Republic of Serbia, No: 171020.*

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Effective ionization coefficients in water vapour

N. Škoro, D. Marić, G. Malović and Z. Lj. Petrović

Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

There is a growing interest for electron interaction data in water vapour owing to several fields of application. One way to obtain such data is from low-current discharges and swarm experiments.

We report on measurements of effective ionization coefficients in water vapour discharge for reduced electric fields (E/N) between 600 Td and 5 kTd. Ionization coefficients shown in Fig.1 are determined directly from experimentally recorded emission profiles of low-current dc discharge. At low pressure, in a low current limit of discharge the electric field is assumed to be homogeneous, with typical exponential rise of emission intensity from the cathode towards the anode. Ionization coefficients are obtained directly from the exponential fit of emission profile [1].

In Fig.1 we also show the results from literature [2,3] for comparison. Our results are systematically lower than others. This could be contributed to a different purity of the water sample, or to a different technique of measurements. In [2] authors obtain ionization an attachment coefficient by fitting Townsend theoretical equation for the current growth to the experimentally obtained current growth in steady state Townsend discharge. In [3] ionization coefficients are obtained from measurements of pre-breakdown currents.

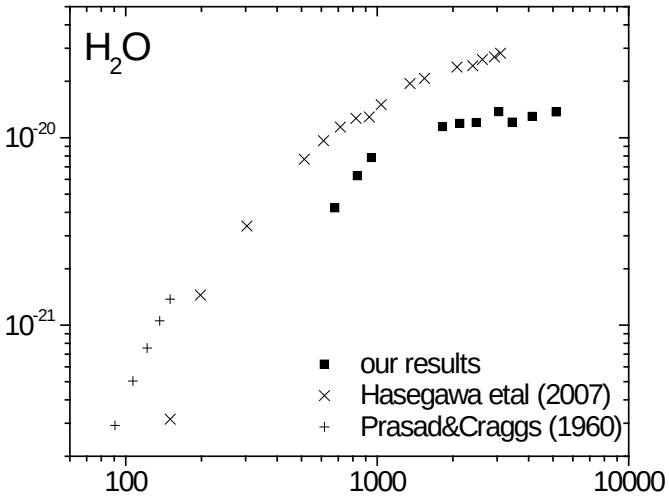

Fig.1. The dependence of reduced ionization coefficient (α/N) on reduced electric field (E/N)

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Detection of atomic species in micro atmospheric pressure discharge by using mass spectrometry

D. Maletić, S. Lazović, N. Puač, G. Malović and Z. Lj. Petrović

Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Large concentrations of radicals, low gas temperatures, absence of vacuum systems and possibility of localized treatment make atmospheric plasmas suitable for modification of sensitive surfaces and for biomedical applications [1, 2, 3]. Here we will present results obtained by mass spectrometry measurements of micro atmospheric pressure plasma jet [4].

Measurements were made for the electron energies below the threshold energy for the dissociation of the O_2 and N_2 molecules (see Fig.1). From these distributions one can identify processes that are pertinent in creation of neutral atoms. In order to eliminate contribution of atoms produced by dissociation of O_2 inside the mass analyzer, the electron energy range was varied from 13.6 eV (required for direct ionization of O) up to 19 eV (less then O_2 dissociation threshold). The counts for atomic O increase with the applied power as well as with the increase in the buffer gas flow. This can be explained by the increase of the electron densities with the applied power. With the increase in the applied power depletion of the molecular oxygen also increases. In case of atomic nitrogen counts stay almost constant with increasing of the applied power.

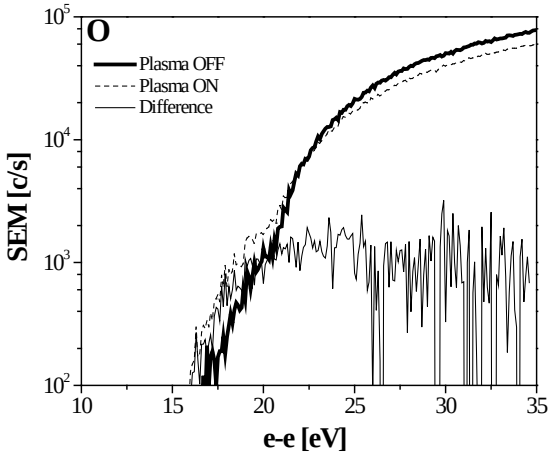

Fig.1. Filament electron energy dependence of oxygen signal (2 slm 1% O_2 70 W).

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Transport properties of positron swarm in molecular nitrogen under the influence of electric and magnetic field

A. Banković[a], S. Dujko[a,b], R. D. White[b], S.J. Buckman[c] and Z. Lj. Petrović[a]

[a]*Institute of Physics, Pregrevica 118, 11080 Belgrade, Serbia*
[b]*ARC Centre for Antimatter-Matter Studies, James Cook University, Townsville 4810, Australia*
[c]*ARC Centre for Antimatter-Matter Studies, Australian National University, Canberra, ACT 0200, Australia*

Low energy positrons are now used in many fields including atomic physics, material science, and medicine [1]. Recent modification of Penning-Malmberg positron buffer-gas trap by Surko and collaborators using a varying configuration of electric and magnetic fields has significantly improved the resolution of low-energy small diameter positron beam [2]. Essentially this apparatus belong to a group of swarm experiments where collisions with buffer gas thermalize the positrons. Further optimization and design of this and similar devices require a detailed investigation of positron transport in neutral gases under the influence of electric and magnetic fields.

Transport properties of positron swarms drifting and diffusing in neutral molecular nitrogen under the influence of crossed electric and magnetic fields are investigated using a multi-term theory for solving the Boltzmann equation [3] and Monte Carlo simulation technique [4]. Molecular nitrogen is of particular importance since it is widely used as a buffer gas in positron traps. In this work, we make a further generalization with respect to our previous publications [5,6] to consider the synergetic effect of non-conservative collisions and the magnetic field on transport coefficients. Values of mean energy, drift velocity, diffusion tensor and rate coefficients are calculated over ranges consistent with practical applications. Transport properties for nitrogen are compared with those obtained for other molecular gases with the aim of determining which gas is the most suitable for applications in collisional positron traps.

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Monte Carlo simulation of RF discharges

M. Savić[a], M. Radmilović-Radjenović[a], M. Šuvakov[a] and Z. Lj. Petrović[a]

[a]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

The mechanism of gas breakdown in radio-frequency (rf) electric fields represents a topic of fundamental [1] and practical importance [2] in the field of low-temperature plasma physics and applications. Capacitively coupled rf discharges are receiving an increased attention due to their wide applications in many technological processes such as plasma etching for semiconductor materials [3], thin film deposition [4] and plasma cleaning [5]. In order to optimize plasma technological processes it is often necessary to know gas breakdown conditions in a discharge device. Therefore, it is of considerable interest to measure and to simulate the rf breakdown voltage curves.

The rf breakdown voltage generally forms a fairly smooth curve with the left hand branch of the curve being markedly steeper than the right hand branch. But, under certain circumstances some changes in the slope of the breakdown curves have been observed [6]. It was found that the left-hand branch of the breakdown curve is a multivalued function of the gas pressure i.e. a single gas pressure corresponds to several breakdown voltages. The multivalued nature of the left-hand branch of the breakdown curve is not explained yet.

This work represents the investigation of the influence of the various parameters (pressure, frequency…) on the breakdown voltage in rf argon discharges. Calculations were performed by using Monte Carlo code developed and tested in our group [6] with well established cross section data for: elastic, two excitations and cross section for ionization [7]. Simulation conditions wee based on the experimental conditions mainly [6]. The obtained simulation results are in a good agreement with the available experimental data [6].

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