CEPAS 2017

7th Conference on Elementary Processes in Atomic Systems

3rd – 6th September 2017

Průhonice, Czech Republic

Table of Contents

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Programme

Sunday, September 3

15:00		Registration
19:00		Opening and welcome reception

Monday, September 4

Photoionization and photoemission - *Chairman: Bratislav Marinković*

9:00	Fernando Martín	Attochemistry: Imaging and controlling electron dynamics in molecules *(Page 9)*
9:45	Ticia Buhr	Azimuth angle dependence of the He 1s and Ne 2s photoelectron angular distributions *(Page 10)*
10:10		Coffee break
10:40	Paola Bolognesi	Radiation damage in systems of biological interest: the case of radiosensitisers *(Page 11)*
11:25	Alexei Grum-Grzhimailo	Coherent control of electron emission in short-pulse XUV atomic ionization *(Page 12)*
11:50	Andrej Bunjac	Calculation of the dynamic Stark shift for sodium and the application to resonantly enhanced multiphoton ionization *(Page 13)*
12:15		Lunch

Electron and photon interactions - *Chairman*: Martin Čížek

14:00	Petr Dohnal	Laboratory study of electron-ion recombination and of associative detachment at low temperatures *(Page 14)*
14:25	Roman Čurík	Inelastic low-energy collisions of electrons with small cations *(Page 15)*
14:50	Petra Votavová	Superexchange Interatomic Coulombic decay by Fano-ADC-Stieltjes method *(Page 16)*
15:15	Viorica Stancalie	Studies of the electron-correlation and relativistic effects in target representation and low-energy collision calculations *(Page 17)*
15:40		Coffee break
16:15		Poster Session, International Scientific Committee meeting
19:00		Individual dinner

Tuesday, September 5

Ion interactions - *Chairman*: Robert DuBois

9:00	Alicja Domaracka	Ion collisions with complex molecular systems: isolated molecules, clusters and astrophysical ices *(Page 18)*
9:45	Sándor Kovács	Dissociative ionization of H_2O molecule bombarded by single charged projectiles *(Page 19)*
10:10		Coffee break
10:40	Jeff Shinpaugh	Experimental and computational study of gold nanoparticles as a radiosensitizer for proton radiation *(Page 20)*
11:25	François Frémont	Classical treatment of autoionization in slow ion-atom collisions *(Page 21)*
11:50	Nikolaus Stolterfoht	Milestones of highly charged ion guiding through insulating cappillaries: applications to a conical sphape *(Page 22)*
12:15		Lunch
14:20		Departure to Prague, Excursion
19:00		Conference Dinner in the Strahov Monastery Brewery

Wednesday, September 6

Electron-impact experiments - *Chairman*: Gustavo García

9:00	Janina Kopyra	Low energy electron driven decomposition of biologically relevant molecules *(Page 23)*
9:45	Marián Danko	Dissociative ionization of cyclopropylamine *(Page 24)*
10:10		Coffee break
10:40	Paulo Limão-Vieira	Decomposition of nitroimidazoles by electron impact *(Page 25)*
11:25	Jaroslav Kočišek	Does pinene stabilize water aerosols? *(Page 26)*
11:50	Nigel Mason	Electron driven chemistry on comet 67P observed by Rosetta space craft and its implications *(Page 27)*
12:15		Lunch
14:00		Departures or individiual afternoon in Prague

List of Posters

Nd:YAG laser ablation of materials of biological interest

M.S. Rabasović[1], D. Sevic[1], B.P. Marinković[1]

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The aim of this study is to analyze the possibilities of using of the Laser Induced Breakdown Spectroscopy (LIBS) for discerning the materials ablated by laser. Lasers are widely used for ablation of biological materials. For practical considerations in biomedical applications, it is necessary to have a real-time feedback control system, so that discriminating between the ablated layers is possible. As excitation laser we use Nd:YAG (1064 nm, pulse width 5 ns, energy up to 300 mJ). We used dry pork bone as an experimental sample. The diagnostic part of our experiment is based on streak camera, so we can perform the time resolved analysis of spectral data. Reasoning of our LIBS analysis follows the concept presented in [1], where femtosecond laser was used for tissue ablation. Sodium (Na) line at 589 nm and Calcium (Ca) line at 612 nm could be used for discrimination between the soft tissue and the bone. Nanosecond Nd:Yag lasers are also widely used for biomedical applications [2,3] Our method of time resolved LIBS is presented in [4]. This study was inspired by a similar analysis (not for biological

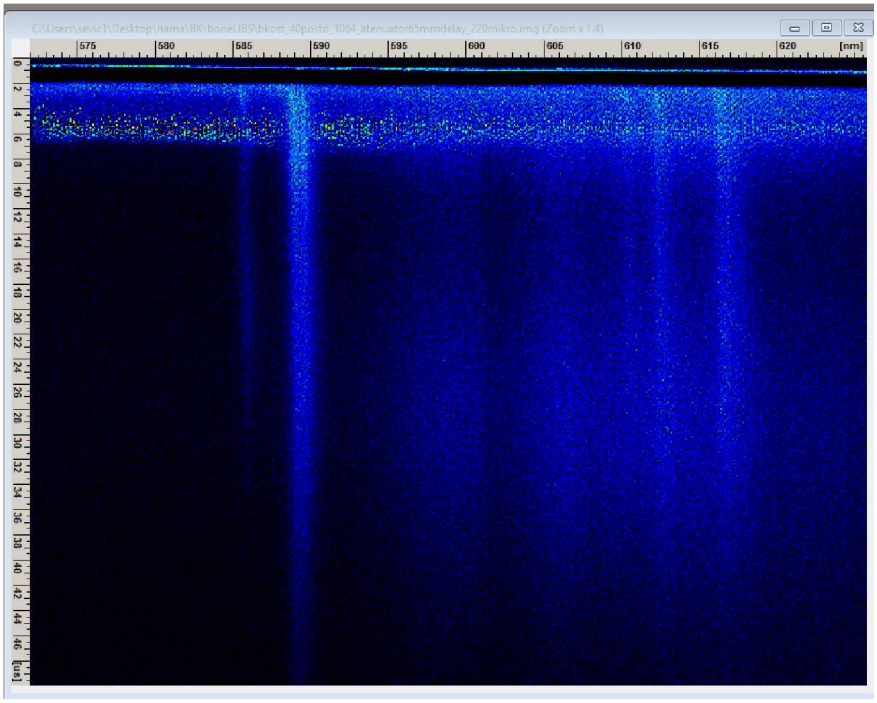

Figure 1: Streak image of LIBS of a dry bone.

materials, but for printed circuit board) presented in [5]. The real application would be based on using the simpler, not time resolved spectrograph with gated acquisition time frame. Our analysis of streak images provides the proof of the concept. Also, the optimal value of gate time is determined by our analysis.

[1] R.K. Gill *et al.*, J. J. Biophotonics **9** (2016) 17.
[2] B. Cencic *et al.*, Appl. Phys. A **112** (2013) 65.
[3] G. Hawlina *et al.*, BMC Ophthalmology **14** (2014) 131.
[4] M.S. Rabasovic *et al.*, IEEE Trans. Plasma Sci. **42** (2014) 2588.
[5] M.S. Rabasovic *et al.*, Appl. Phys. A, **122** (2016) 186.

Ejected electron spectra from Coster-Kroning transitions in argon

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[2]*CNR-Istituto di Struttura della Materia, Area della Ricerca di Roma 1, CP10, 00015 Monterotondo Scalo, Italy*

High resolution ejected electron spectroscopy has been used to investigate ejected electrons in the energy region of the Coster-Kronig (C-K) transitions from 25 to 56 eV in Ar at incident electron energies of 243, 324, 606, 909 and 2018 eV and fixed ejection angle of 90°. The C-K spectrum in Ar includes transitions from the initial state $1s^2 2s 2p^6 3s^2 3p^6$ to the final states $1s^2 2s^2 2p^5 3s(^1P,^3P)3p^6$, and $1s^2 2s^2 2p^5 3s^2 3p^5(^3D, ^1D, ^3S, ^1S)$ [1]. In the C-K process the vacancy in the 2s shell (L_1) made by the impact of electrons with energies larger than 327 eV is filled by an electron from the 2p subshells ($L_{2,3}$), while the second electron from either 3s or 3p subshells (M_1, $M_{2,3}$) is promoted to the continuum. The final result is formation of two separate groups of peaks around 30 and 50 eV i.e. (L_1-$L_{2,3}M_1$) and (L_1-$L_{2,3}M_{2,3}$) respectively.

The intensity evolution of all states in the C-K energy region was studied at several incident electron energies from 243 to 2018 eV. The calibration of ejected energy scale was made with respect to the energy position of the Ar 3d(^{1}D) state at 11.72 eV measured under the same experimental conditions.

The measurements have been carried out using a crossed electron-atom beam apparatus OHRHA [2] equipped with an electron gun that can be rotated around the axis of the electrostatic lenses of the analyzer, and the hemispherical analyzer with 7 channeltrons as detectors. The energy resolution of the ejected electron spectra measured as full width at half maximum (FWHM) of the narrowest feature in the spectrum, was typically between 60 and 80 meV.

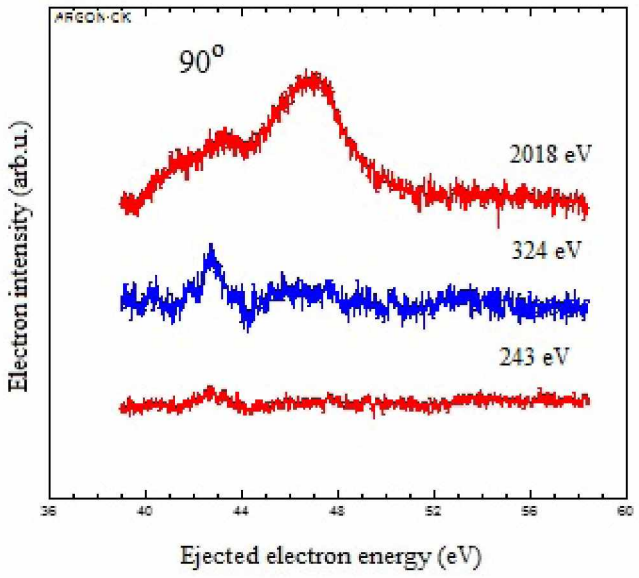

Figure 1: Coster – Kroning transition lines in Ar obtained at 243, 327 and 2018 eV incident electron energies and ejection angle of 90°.

[1] T. Kylli *et al.*, Phys. Rev. A **59** (1999) 4071.
[2] J.J.Jureta *et al.*, Int.J.Mass Spectrom. **114** (2014) 365.

Electron transmission through steel capillary

B.P. Marinković[1], M.Lj. Ranković[1], J.B. Maljković[1], A.R. Milosavljević[2], D. Borka[3], C. Lemell[4], K. Tökesi[5]

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The transmission of low-energy electrons through platinum [1, 2] and steel capillaries have been investigated both experimentally and theoretically. The length of the present steel capillary was $L = 19.50$ mm while the inner diameter was $d = 0.90$ mm. Kinetic energy distribution of electrons transmitted through steel capillary was recorded at two tilt angles (the angle between the incident electron beam and the capillary axis) of 2.64° and 4.0°, respectively. The experimental results were obtained by an electron spectrometer which consists of an electron gun, a double cylindrical mirror energy analyzer (DCMA) and a channeltron detector.

Electron transmission is modelled by a classical trajectory Monte Carlo simulation taking both elastic and inelastic scattering events of primary electrons colliding with the inner wall of the capillary and transport of secondary electrons into account.

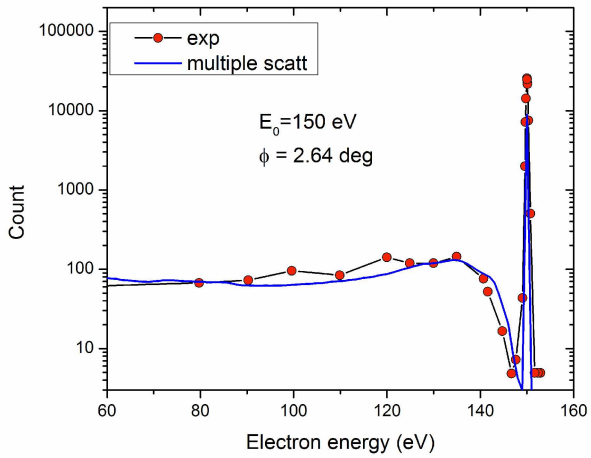

Figure 1: Energy spectra of electrons transmitted through a steel capillary.

Figure 1 shows energy spectra of 150 eV electrons passing through the steel capillary at 2.64° tilt angle. We found excellent agreement between our simulated electron-energy spectra with experimental data.

[1] A.R. Milosavljević *et al.*. Nucl. Instr. Meth. Phys. Res. B **354** (2015) 86.

[2] D. Borka *et al.*, Nucl. Instr. Meth. Phys. Res. B, in press (2017), http://dx.doi.org/10.1016/j.nimb.2017.02.024

High resolution study of the autoionizing states of He in the vicinity of the equal velocity region

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By "equal velocity region" we mean the primary electron energy range in which the energies of the autoionizing electrons approximately match that of the scattered electrons. This range is around 90-95 eV for the four most important autoionizing states of helium. Then such interesting phenomena can occur as the post-collision interaction and certain types of the state-to-state interference. We have been studying this range for a long time [1], concentrating the interference of the $2s^2(^1S)$ and $2p^2(^1D)$ resonances. It takes place at 93.15 eV critical primary energy, where the energy of the scattered electron from one reaction path equals the energy of the ejected (autoionizing) electron released along the other path and vice versa: here the scattered-ejected electron pairs are indistinguishable. The observation of this exchange interference is disturbed by the Fano interference (the interference between the direct and indirect ionization), too, which occurs at all primary energies. We intend to study it separately in the neighbourhood of the critical energy, and then to estimate its measure for the critical energy.

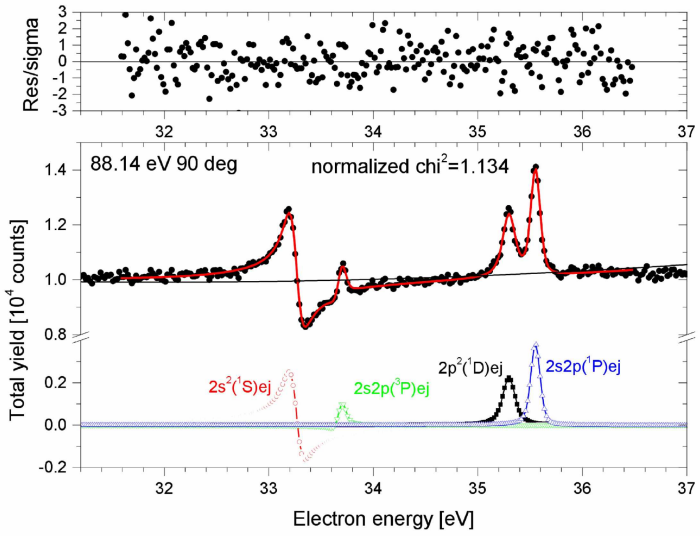

Figure 1: The electron spectrum measured at 90° ejection angle at 88.14 eV primary energy with the best computer fit (solid line). At the bottom the spectrum components, at the top the residuals (in sigma units) are shown.

The present measurements were made by an Omicron High Resolution Hemi-spherical Analyzer (OHRHA) [2] at 88 eV and 97 eV primary energies (where the groups of the ejected and the scattered electron peaks are well separated), at 130°, 90° and 50° ejection angles. The measured spectra were evaluated by a computer code, using the Shore parametrization.

[1] B. Paripás *et al.*, Eur. Phys. J. D **69** (2015) 34.
[2] J.J. Jureta *et al.*, Int. J. Mass Spectr. **114** (2014) 365.

The photofragmentation of the core excited halothane molecule

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In recent years, great attention has been paid to halogenated anesthetics and their role in the destruction of the earth's ozone layer [1]. One of the most commonly used is halothane ($C_2HBrClF_3$). Compared to the other volatile anestethics from the same group (halogenated chlorofluorocarbons) this bromide-containing agent is the most destructive against ozone.

We present both experimental and theoretical results related to the photofragmentation of the core-excited halothane molecule. The experiments have been performed at the Gas Phase photoemission beamline of the Elettra synchrotron radiation source (Trieste, Italy) using photons near the C 1s ionization edge ($\sim$ 300 eV). The mass spectrum [as shown in Fig.1] is dominated by lighter mass fragments.

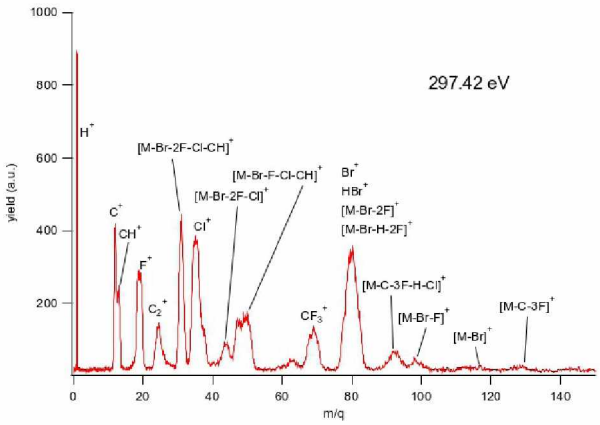

Figure 1: The fragmentation mass spectra of halothane.

To explain the observed large number of lighter mass fragments extensive molecular dynamics (MD) simulations of $C_2HBrClF_3^{2+}$ ion at different temperatures were performed. All MD simulations were carried out in the microcanonical (NVE) ensemble using Verlet algorithm for time integration. At each step of the simulation the potential energy was calculated by minimizing the electronic energy with self-consistent charge-density-functional tight-binding (SCC-DFTB) method as implemented in the DFTB+ code [2]. The results of MD simulations have confirmed the experimental findings: there are fragmentation paths producing almost all fragments found in the mass spectra. For the main fragmentation pathways the minima and the transition states on the potential energy surface were calculated with more accurate quantum chemical methods.

Work partially supported by the MAECI Serbia–Italy Joint Research Project "A nanoview of radiation-biomatter interaction" and the MESTDRS (OI 171020, OI 172065).

[1] A.C. Brown *et al.*, Nature **341** (1989) 635.
[2] B. Aradi *et al.*, J. Phys. Chem. A **111** (2007) 5678.