

МІЖНАРОДНА КОНФЕРЕНЦІЯ

Резонансні явища в атомних системах

(до 85-річчя академіка НАН України Отто Шпеніка)

19-21 вересня 2023 року

НАУКОВІ ПРАЦІ



INTERNATIONAL CONFERENCE

Resonance Phenomena in Atomic Systems

(to the 85th anniversary of Academician Otto Shpenik)

September 19-21, 2023

**Інститут електронної фізики НАН України
ДВНЗ «Ужгородський національний університет»**



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Збірник наукових праць містить матеріали та тези доповідей, представлених на Міжнародній конференції «Резонансні явища в атомних системах». Конференція присвячена 85-й річниці від дня народження Отто Бартоломійовича Шпеніка - відомого українського вченого, провідного спеціаліста в галузі фізики електронних і атомних зіткнень, одного із засновників фізичної школи з атомної фізики на Україні, першого директора Інституту електронної фізики НАН України, академіка НАН України, іноземного члена Угорської академії наук. У доповідях представлені результати досліджень резонансних явищ при електронних і атомних зіткненнях, елементарних процесів у лазерах і низькотемпературній плазмі, спектроскопії атомів і молекул, ядерній, радіаційній та теоретичній фізиці.

The collection of scientific works contains materials and abstracts of reports presented at the International Conference "Resonance Phenomena in Atomic Systems". The conference is dedicated to the 85-th anniversary of the birth of Otto Shpenik, a well-known Ukrainian scientist, a leading specialist in the field of physics of electronic and atomic collisions, one of the founders of the physical school of atomic physics in Ukraine, the first director of the Institute of Electronic Physics of the National Academy of Sciences of Ukraine, an academician of the National Academy of Sciences of Ukraine, a foreign member of the Hungarian Academy of Sciences The reports are devoted to the study of resonance phenomena during electronic and atomic collisions; elementary processes in lasers and low-temperature plasma; spectroscopy of atoms and molecules, nuclear, radiation and theoretical physics.

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ELECTRON EXCITATION OF CADMIUM METAL ATOM RESONANCE LINE

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1. INTRODUCTION

The idea of this mini review is to cover studies done on electron interactions with cadmium atom, preferably having in focus the resonance line and its excitation by slow electron beams. In some more detail the investigations performed in Belgrade and Uzhhorod are highlighted.

Electron interactions with atoms and molecules at low (below 10 eV or the corresponding ionization potential) and intermediate energy range (10-100 or up to 1000 eV) have been in constant focus since the discovery of electron in 1897 (cf. [1,2]). However, studies of electron scattering by metal atoms are not so frequent, especially experimental ones, since they require sophisticated experimental equipment. Contrary to the energy-loss spectra of rare gas atoms where the elastic scattering peaks dominate over all excitations (e.g., in argon the intensity ratio of elastic-to-inelastic noticeable peak spans in one to two orders of magnitude [3]), the energy-losses of metal atoms are dominated by the resonance line that is usually the first optically allowed state. Prominent examples are sodium and cadmium atoms, the first one dominated by the excitation of the $3^2P_{1/2,3/2}$ state (Fig.1 in [4], note that the resolution in electron spectra which is usually of the order of 10 meV would not allow one to separate fine structure), while in the case of cadmium it is the 5^1P_1 line (Fig.7 in [5] where the resonance line is preceded by the optically forbidden lines $^3P_{0,1,2}$).

Since cadmium is widespread in soil and groundwater [6] and is a recognized contaminant of food and biological tissues [7], it has been a constant objective in many studies. Singly charged cadmium ions have been found in the gas-phase interstellar clouds [8], while Cd IV lines were detected in the near-infrared emission spectra of planetary nebulae [9].

Cadmium is a chemical element with atomic number 48, as a metal it belongs to the group 12, period 5 of Periodic System. Its melting point is below 600 K and its vapors are very poisonous. Electron configuration of the ground state is $[\text{Kr}]4d^{10}5s^2$.

2. ELECTRON SCATTERING BY CADMIUM ATOM

2.1. *STUDIES OF e/Cd at the IEP UZHGOROD*

Electron interactions with cadmium atom and ions have been investigated since the first constructions of experimental set-ups with monoenergetic electron beams at the Institute of Electron Physics, Uzhhorod [10] where resonance effects in inelastic collisions of slow electrons with cadmium [11] have been investigated in detail. Using the crossed-beam method and a hypocycloidal electron spectrometer (HEM), the energy dependence of the ionization cross section for the cadmium atom has been studied in the near-threshold region as well as the elastic scattering of slow electrons [12]. The same authors measured total cross sections up to 15.3 eV where they have identified the $5s^25p\ ^2P$ resonance structure at the energy of 0.35 eV as well as the resonance feature near the $5\ ^3P_{0,1,2}$ levels of cadmium [13]. Additionally, total cross sections for the excitation of the 5^1P_1 state and averaged total cross sections for the $5\ ^3P_{0,1,2}$ levels from the corresponding thresholds to 11 eV have been presented in absolute scale [13]. Elastic cross sections for e/Cd were determined up to 6 eV together with total cross sections and electron transmission curves at discrete angles from 24° up to 180° revealing distinct shape resonances in the near-threshold region [14].

By using an ultra-monoenergetic electrons emerging from HEM, the precision measurements of optical excitation functions for 14 spectral lines of the cadmium atom originating from the n^1S_0 , 5^1P_1 , n^3S_1 , 5^3P_1 , and n^3D_J levels [15] were done. Performing R-matrix calculations of the cross sections for the excitation of cadmium Cd^+ ion by low-energy electrons, many resonance structures have been obtained strongly influenced by the 4d sub-valence shell [16]. In a crossed electron/atom beam by means of the optical method the energy dependence of the absolute excitation cross sections from metastable cadmium atoms were obtained [17]. The transitions from the $5\ ^3P_{0,1,2}$ levels to the $6\ ^3S_1$ level (wavelengths are 467.8, 480.0 and 508.6 nm, respectively) as well as the transitions from the $5\ ^3P_2$ level to the $5\ ^3D_J$ and $6\ ^3D_J$ levels (at 361.4 and 298.2 nm, respectively) were measured and absolute cross section values were determined.

Other studies on cadmium atom include excitations in slow ion-atom collisions [18,19] performed in early seventies. Here, new apparatus had been utilized for collisions of slow zinc atoms by cadmium and optical excitation functions were recorded, showing fine-structure maxima on most of the 13 measured spectral line curves [18]. In [19] a series of collisions of slow alkali and alkali-earth cations with

cadmium have been studied in the energy range from threshold to 1000 eV and cross sections have been determined for excitation of a number of lines of the target atoms.

A series of studies on the mechanisms of the electron-impact excitation of cadmium cations were performed in order to shed light on the excited level population in helium–cadmium lasers [20]. The role of autoionizing states in this kind of processes [21,22] or processes involving dielectronic recombination [23,24] were further examined in more recent papers. Post-collision interaction upon electron excitation of Cd 1S and 3D lines was studied by optical excitation functions for two series of spectral lines [25]. The excitation functions of three spectral lines originating from the $5snp\ ^1P_1$ levels ($n = 6, 7, 8$) have been recently measured showing the manifestation of the post-collision interaction and the decay of autoionization states [26].

2.2. STUDIES OF e/Cd at the IPB BELGRADE

A detailed review of work performed on metal atoms by colleagues from IPB till 2010 was presented at the conference proceeding [27]. At the Institute of Physics Belgrade (IPB) we utilized an electron spectrometer with hemispherical monochromator and analyzer (Figs.1,2) especially designed for crossed electron/metal atom beam studies [28]. Among the first metal targets was cadmium atom [5], followed by distorted-wave calculations [29].

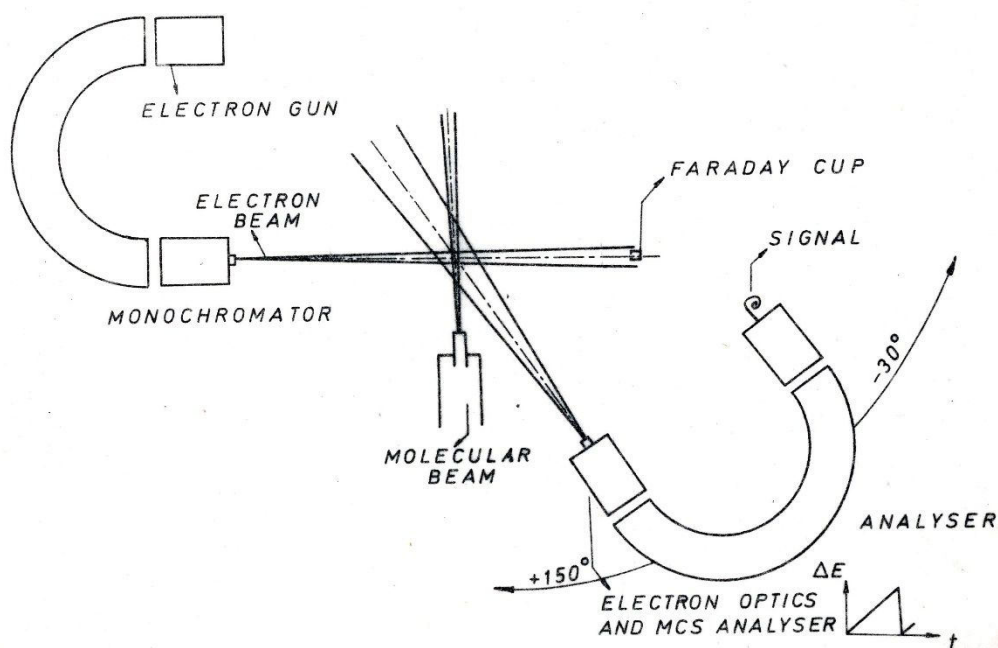


Figure 1. Schematic drawing of electron spectrometer ESMA at the IPB



Figure 2. Photos of electron spectrometer ESMA at the IPB showing vacuum chamber and electronics as well as the inside vacuum chamber

In brief, electron spectrometer ESMA consists of hemispherical monochromator and analyzer with radii of the outer and inner hemispheres of $R_1 = 65.5$ and $R_2 = 34.1$ mm, respectively, accompanied by electrostatic lenses for accelerating, deaccelerating and focusing electron beam with parameters described in detail in [30]. The scattering angle can be varied by rotating the analyzer about the atomic beam axis while the electron monochromator remains in the same position so that scattered electron intensity can be measured from -30° up to $+150^\circ$. All the external electric and magnetic fields are minimized so that the residual magnetic field inside the chamber was reduced by a double μ -metal shield to less than 0.1 pT. The oven of Knudsen type is made of stainless steel, the crucible containing 99.95% pure cadmium that effuses as a beam through a channel 1.1 cm long and 0.15 cm in diameter [5]. Operating temperature was 580 K, corresponding to a vapor pressure of 8 Pa. The nozzle was maintained at a temperature 50 K higher in order to prevent clogging and to minimize dimer production.

The main problem in determination of cross sections of electron scattering by metal atom is how to obtain the absolute scale. For the gaseous targets that effuse from (micro)capillaries, the method of relative flow (cf. [31] and references therein) has been demonstrated and the cross sections for known gas (usually He or Ar [32]) are compared with the target gas, providing certain conditions of equal flow for both gases. The procedure of obtaining the absolute DCS values from the relative experimental data points for metal atom vapors has been given in [28]. The relative differential cross sections (DCSs) for the 5^1P_1 excitation are measured at small scattering angles from 1° to 10° in 1° increments and between 10° and 150° in 10° increments. These relative DCSs were converted to generalized optical oscillator strengths (GOS) that are

extrapolated towards optical oscillator strength (OOS) in the limit of zero momentum transfer. A procedure has been developed by Lassette [33] and further refined in [34]. For the optical oscillator strength of the 5^1P_1 state the value of 1.41 obtained in [35] was used, while the theoretical relativistic convergent close-coupling (RCCC) data are used to extrapolate the DCS to backward scattering angles.

Integral elastic cross sections were obtained from the separate set of intensity ratio measurements of DCSs for elastic and 5^1P_1 excitation at the scattering angle of 20° for 20 eV and lower energies and at 10° for 40 eV and higher impact energies. The transmission of the electron analyzer has been obtained experimentally, and it has been taken into account for every impact energy. This procedure gives an absolute uncertainty of 35% for the measured integral elastic cross sections [36].

The autoionizing states of cadmium have been measured at the IPB in 2003 [37] where the electron-impact excitation cross sections of the 5^3P_1 (12.062 eV) and 5^1P_1 (12.810 eV) $4d^95s^25p$ autoionizing states of Cd were obtained at incident electron energies from 15 to 60 eV. The absolute DCSs at 40 eV were determined through normalization to the OOS. The values for OOS of 0.07 for the 5^3P_1 state and 0.53 for the 5^1P_1 state were adopted from photo-absorption measurements [38]. Energy-loss spectra for Cd were recorded from 11 to 18 eV, and 22 autoionizing states were identified at different impact energies. For the unresolved feature near 12.81 eV, which contains 5^1P_1 and 5^3D_1 states, a decomposition into two log-normal profiles was performed.

In Fig.3 current IPB measured integral cross sections for electron excitation of the 5^1P_1 state with corresponding uncertainties in the energy range from 6.4 to 85 eV together with recommended cross sections are presented. Data points are those published in [36].

2.3. OTHER STUDIES OF CADMIUM AND ITS RESONANCE LINE

Studies of electron interactions by cadmium atom at other worldwide centers are also existing. At University of Southampton 5^1P_1 GOS were determined in the incident electron kinetic energy in the range 60-150 eV [39] as well as high-resolution ejected-electron spectrum of cadmium autoionizing levels following two-electron excitation by low-energy electron impact [40] and spectra at intermediate energy range from 15 to 400 eV [41]. At the University College London experimental study on elastic electron scattering by Cd was performed [42], while at the Roorkee [43], Livermore [44] and Ohio [45] the phase shifts and DCSs for the same process have been calculated. More recently at University of Rajshahi solving the relativistic Dirac

equation and using an optical model potential elastic cross sections have been determined in the broad range of energies, up to GeV [46].

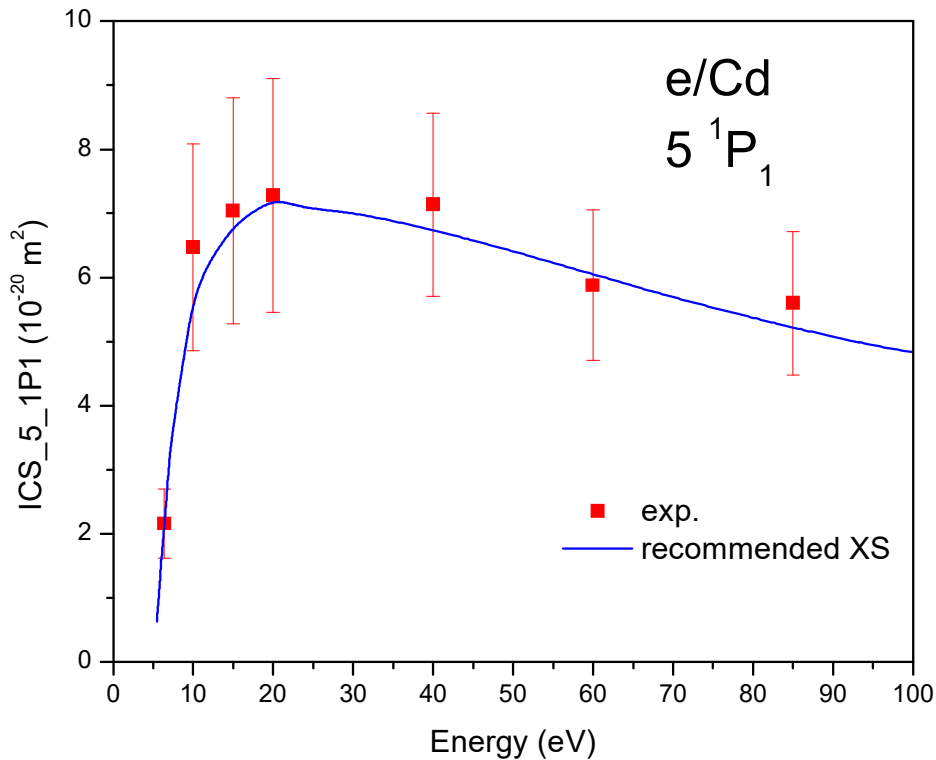


Figure 3. Absolute integral cross sections for the excitation of the resonance Cd line 5^1P_1 : Measured CS data with the uncertainties (squares); RCCC calculation and recommended CS (full curve). Data points are those published in [36]

An experimental and theoretical study of transient negative ions in cadmium and some other metal atoms have been published by Australian group [47]. At Yale they have measured electron scattering at low energy from Cd using the electron transmission method and have observed large shape resonance identified with the ground state of the negative ion [48]. This has been recently confirmed by semiempirical calculations performed in Florianópolis, Brazil [49]. Spin polarization of elastically scattered low energy electrons was calculated in Gdańsk [50], while a series of polarization measurements for the excited state have been performed in Toruń [51] accompanied with the studies of the electron impact coherence parameters and reduced Stokes parameters for excitation of the 5^1P_1 state [52].

At Cheboksari measurements of relative cross sections for electron super-elastic scattering from the 5^3P_1 state of Cd atoms with slow electrons were done in the energy range of from 0.6 eV to 4 eV [53]. Atoms were excited by optical pumping from an external light source. The autoionizing states of cadmium have been studied as well

from early eighties [54]. In 1981 new resonances in the cross sections for e/Cd scattering were found [55].

A series of experiments with cadmium vapor have been employed at the University of Kentucky during nineties. Also, a theoretical analysis of photo-absorption cross section in the $\text{Cd } 4d^9 5s^2 5p$ autoionizing resonance region has been re-analyzed using overlapping resonance theory [56]. This led to different assignment of the main peaks in this region, previously thoroughly analyzed by Mansfield and Murnane [57]. The $(e, 2e)$ energy spectra in cadmium for the $4d^9 5s^2 5p J=1$ autoionizing region were obtained in [58] with the investigated ejected-electron energy range from 2.6 to 4.8 eV and the incident electron energy of 150 eV and a scattering angle of 3° . There, the interference terms arising from coherent excitation of the $J = 1$ and overlapping $5pnp J = 0, 2$ autoionizing levels were found and explained [58,59]. Further investigation of complex ionization amplitudes in cadmium by $(e, 2e)$ spectroscopy led to the conclusion that both resonant and non-resonant processes are important when one is considering relative magnitudes and phases of ionization amplitudes [60]. In order to minimize spreading of cadmium vapor within vacuum chamber due to relatively small sticking coefficient, it was necessary to design the efficient trap [61]. New analysis of $(e, 2e)$ angular distributions and energy spectra unified previous data sets from [41] and these new measurements giving the plausible explanation taking into account the asymmetry parameter and contribution of direct ionization for all J partial waves [62]. A technique of the normalization of ejected-electron spectra using Auger peaks was presented in [63]. Measurements have been extended towards the observation of $\text{Cd } 4d^9 5s^2 5p J=3$ autoionizing levels in $(e, 2e)$ energy spectra [64]. A variation of kinematic parameters in $(e, 2e)$ ejected electron spectra led to the conditions of dipole limit to the binary collisions' regime [65].

A group from Perth and Toronto have performed extensive calculations of electron scattering from the ground state of cadmium atom using the convergent close-coupling, relativistic convergent close-coupling, relativistic optical potential, and relativistic distorted-wave methods [66]. They calculated elastic and inelastic differential cross sections, Stokes parameters, and spin-asymmetry parameters.

2.4. RECOMMENDED CROSS-SECTIONS FOR e/Cd

While the recommended cross sections for positron scattering by cadmium atom has been published [67]; however, the same kind of recommendation has not existed for electrons up to recently. Most recently a new comprehensive experimental and theoretical study on electron scattering by cadmium have been presented by a group of

authors [36]. Here, the measurements of integral cross sections are presented for elastic scattering and for the excitation of the 5^1P_1 state. Integral cross sections for elastic scattering, summed discrete electronic-state excitation, and ionization scattering processes are calculated over an extended incident electron-energy range using several different approximations: optical potential, relativistic optical potential, relativistic convergent close-coupling, and binary encounter Bethe models. Total cross sections are constructed by taking their sum. Recommended electron cross-section datasets are given over an incident electron energy range from 10^{-2} to 10^{+4} eV.

In Fig.4 current IPB measured integral cross sections for elastic electron scattering with corresponding uncertainties in the energy range from 6.4 to 85 eV together with recommended cross sections are presented. Data points are those published in [36].

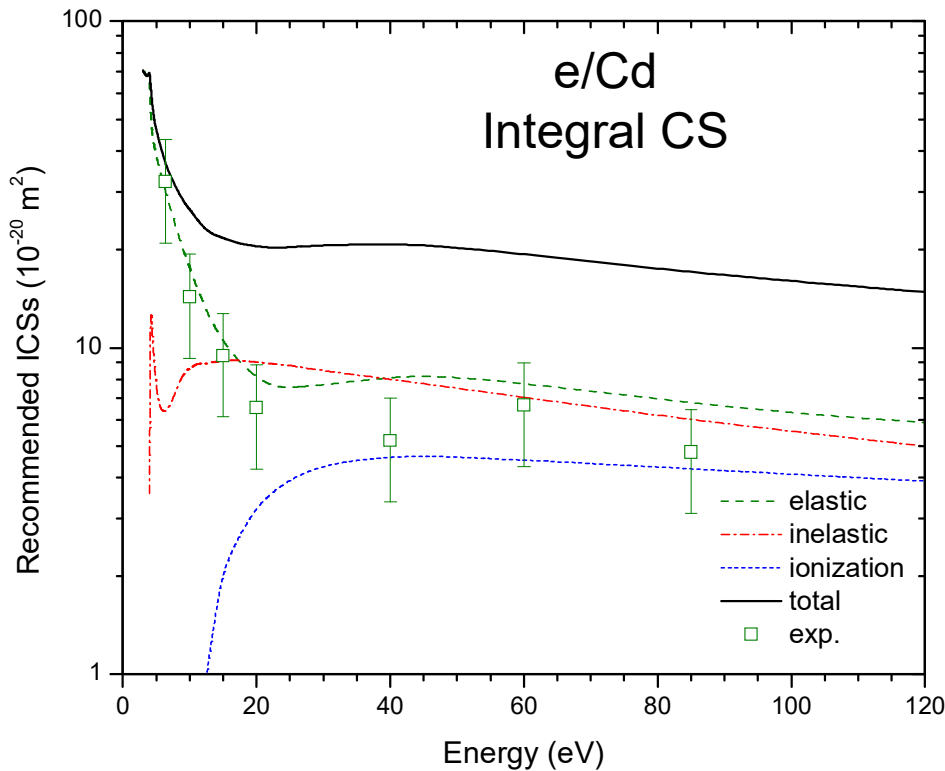


Figure 4. Recommended integral cross sections for the elastic (dash), inelastic (dash-dot), ionization (short dash) and total (full curve) scattering and measured elastic cross section data with the uncertainties (open squares). Data points are those published in [36]

3. CONCLUSIONS

Electron scattering by cadmium atoms has been of constant interest at many laboratories across the world since the first measurements by Childs and Massey [68]

in 1933 and up to current year when the recommended integral cross sections have been published for elastic, inelastic, ionization and total electron scattering [36]. These cross sections have found their place in atomic and molecular data bases, such is the wide spread VAMDC (Virtual Atomic Molecular Data Centre) and one of its nodes BEAMDB [69]. Reliable data of cross sections can provide a good foundation for modelling purposes and other application.

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