

PRECISE EXPERIMENTAL AND THEORETICAL STUDIES ON RESONANT ENERGIES OF THE KLL DIELECTRONIC RECOMBINATION PROCESSES FOR HE- UP TO O-LIKE XENON

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Dielectronic recombination (DR) is a resonant process, in which a free electron is captured by an ion, and at the same time a bound electron of the ion is excited, followed by radiative stabilization. Studies of DR processes are very important, not only for researches relevant to hot plasmas, but also for atomic structure and collision theory, as DR processes carry information on quantum electrodynamics, relativistic effects, many body interactions and so on.

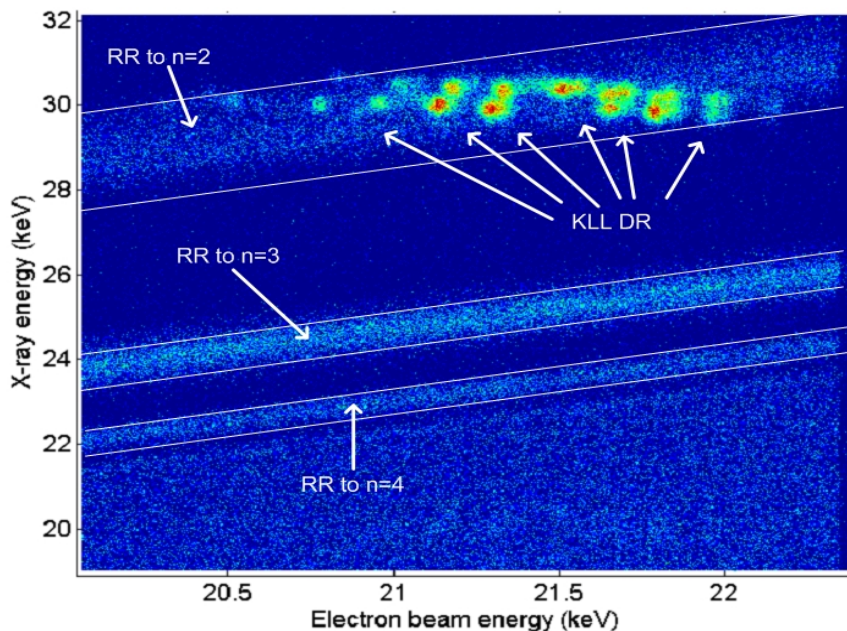


Fig. 1: Scatter plot of X-ray counts over electron beam energy and photon energy, taken at electron beam current of 62 mA. The KLL DR resonant events and radiative recombination to $n=2, 3, 4$ are shown.

Precise experimental studies of the resonant energies of KLL DR processes of He-, Li-, Be-, B-, C-, N-, and O-like xenon ions were performed at the Shanghai Electron Beam Ion Trap, by monitoring the electron beam energies over the KLL DR resonance region, see Fig. 1, employing home developed high precision, high stability high voltage dividers. Effects of the space charge of the electron beam and the ion neutralization, retardation by the capacitor of experimental setup, contact potential as well as fringing field effects were taken into account. Fifteen experimental resonant energies were obtained at an average uncertainty level of 0.03%.

At the same time, calculations using relativistic configuration interaction (RCI) theory, relativistic many-body perturbation (RMBPT) theory were also performed for the above-mentioned KLL DR resonant energies. Comparisons of experimental and theoretical results were made. 13 out of the 15 predictions by RMBPT are in good agreement with our experimental results, while only 5 out of the 15 predictions by RCI calculation agree with our experiments. Three literature available DR resonant energies by multi-configuration Dirac-Fock calculation agree very well with our experiments.

ANGLE-RESOLVED STUDIES OF HYPERSATELLITE RADIATION FOLLOWING DIELECTRONIC RECOMBINATION OF HEAVY IONS

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In the process of dielectronic recombination a free (or quasi-free) electron is resonantly captured by an ion under the simultaneous excitation of an ionic electron. For many years, such an electron capture has been of great interest both, for experiment and theory since it occurs frequently in high temperature plasmas. Apart from the plasma studies, dielectronic recombination (DR) is also playing an important role for understanding the interelectronic interaction effects. In order to explore these effects in heavy atomic systems, a number of DR experiments have been carried out recently for relativistic collisions of highly-charged projectile ions and target electrons at ion storage rings. At the GSI storage ring in Darmstadt, for example, $K - LL$ dielectronic recombination of (finally) helium-like uranium U^{90+} ions and their subsequent radiative decay have been studied in detail [1]. While measured data were generally well understood within the Dirac's relativistic theory [2], a considerable discrepancy was found for the angular distribution of the $K\alpha_1$ hypersatellite radiation following the $K - L_{1/2}L_{3/2}$ resonant electron capture [1,2].

In the present work, we apply the density matrix theory together with the multiconfiguration Dirac-Fock method in order to re-investigate the dielectronic recombination of (initially) hydrogen-like ions and their subsequent radiative decay. Special emphasis is placed on the characteristic x-ray emission whose angular distribution may be modified by higher (non-dipole) terms in the expansion of the electron-photon interaction. In particular, we show that the emission pattern of the hypersatellite $K\alpha_{1,2}$ lines is notably influenced by the interference between the leading electric dipole $E1$ and — the much weaker — magnetic quadrupole $M2$ decay channels [3]. Detailed calculations for such a multipole-mixing phenomena are performed for the decay of the doubly-excited LL resonances of U^{90+} ions and are compared with the previous experimental [1] and theoretical [2] data.

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PHOTORECOMBINATION OF SODIUMLIKE SILICON IONS: ASTROPHYSICALLY MOTIVATED STORAGE RING EXPERIMENTS AND MCDF CALCULATIONS

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The origin of large-scale structure in the universe, the history of star and galaxy formation, the metagalactic radiation field, and the chemical evolution of the intergalactic medium (IGM) can be studied by the use of spectroscopic observations of absorption lines in the IGM (see [1] and references therein). Coupled with calculations of the ionization balance, these observations provide important constraints for IGM studies.

However the accuracy with which one can infer the properties of the IGM is limited by uncertainties in the underlying atomic data. Of particular importance are reliable electron-ion recombination data for the process known as dielectronic recombination (DR). This is the dominant recombination process for most ions under IGM conditions. Recent investigations [2] have shown that uncertainties in the DR data for C IV, N V, O VI, and Si IV limit the ability to constrain the metagalactic radiation field and the initial mass function for the earliest generations of stars.

This situation has motivated us to measure the Si IV to Si III recombination rate coefficient employing the electron-ion merged-beams method at the Heidelberg heavy-ion storage ring TSR. The measured electron-ion collision energy range of 0–186 eV comprises DR resonances associated with $3s \rightarrow 3p$, $3s \rightarrow 3d$, $2p \rightarrow 3l$ and $2p \rightarrow 4s$ excitations. The present experimental Si IV merged-beams recombination rate coefficient allows us to benchmark theory for a light, low charged sodium-like ion over a wide range of energies.

The present study is complemented by calculations of DR cross sections and rate coefficients based on the multiconfiguration Dirac-Fock (MCDF) method, in particular at low electron-ion collision energies. At these energies the calculation of accurate resonance positions and strengths is most critical for the derivation of accurate plasma rate coefficients [3]. Our experimental results are compared with other experimental and theoretical results [4].

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EXPERIMENTAL RATE COEFFICIENT FOR DIELECTRONIC RECOMBINATION OF NEONLIKE IRON FORMING SODIUMLIKE IRON

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Emission lines from highly charged iron ions are prominent in the high resolution x-ray spectra from many astrophysical objects as has been observed, for example, with the x-ray telescopes CHANDRA and XMM-NEWTON [1]. The $\text{Fe}^{16+} 2p^6 - 2p^5 3s$, $2p^6 - 2p^5 3d$, and $2p^6 - 2p^5 4d$ lines in the 12–17 Å wavelength range are strong emission features of many coronal sources. Interpreting the emission from these lines depends partly on accurately knowing the underlying ionization balance of the emitting gas.

One of the important processes for determining ionization structure is dielectronic recombination (DR) which is the dominant electron-ion recombination mechanism for most ions in cosmic plasmas. Over the last few years a number of groups have systematically calculated DR cross section and plasma rate coefficients for ions with an open K- and L-shell (see [2] for an overview). But these results for Ne-like ions can differ up to 140% depending on the ion species and the plasma electron temperature [2].

In our ongoing effort of providing reliable DR rate coefficients for astrophysical applications (see e. g. [3, 4]) we have measured the DR rate coefficient of Ne-like Fe^{16+} forming Na-like Fe^{15+} employing the merged electron-ion beams technique at the heavy-ion storage ring TSR of the Max-Planck-Institut für Kernphysik in Heidelberg, Germany.

The present experiment is the first merged-beams measurement for an ion of the Ne-like isoelectronic series and, therefore, represents an important benchmark for theoretical calculations. We find good agreement between our experimentally derived rate coefficient in a plasma and recent theoretical results [5, 6].

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Evaluation of direct ionization cross sections for C_{60} by electron interaction

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Electron interaction with fullerenes like C_{60} has a growing interest in the present time due to its manifold applications. Despite many experimental and theoretical studies about the collisional interaction between electrons and fullerenes, so far there exist only a few absolute electron impact ionization cross sections measurements of C_{60} . This is generally due to the great difficulty in calibrating measured relative cross section functions, which requires, among other pre requisites, as a quantitative knowledge of target and ionizing electron beam. In the present study, we have extended a previously developed semi empirical method [1-2] for the calculation of ionization cross sections corresponding to the formation of singly charged ions C_{60}^+ , doubly charged ions C_{60}^{++} and triply charged ions C_{60}^{+++} in electron- C_{60} collision. The calculations are made in the energy range varying from ionization onsets to 1 KeV. The major input, required oscillator strengths are used from the recent established experimental measurements of Jaensch and Kamke [3], Reinköster et.al. [4] and Berkowitz [5]. The calculated cross sections shown in the figure compare well with the experimental data of Märk et al. [6].

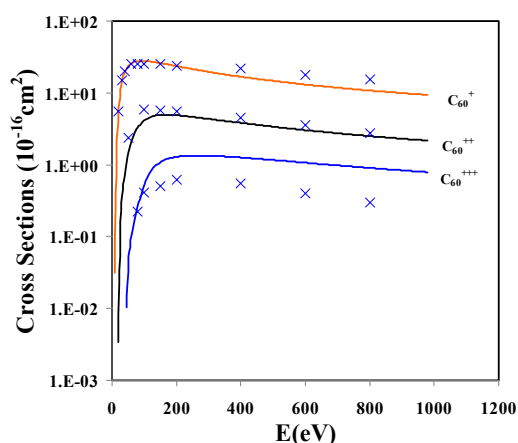


Figure: Electron impact ionization cross sections (designated by solid lines) in comparison with the experimental data designated by \times [6]

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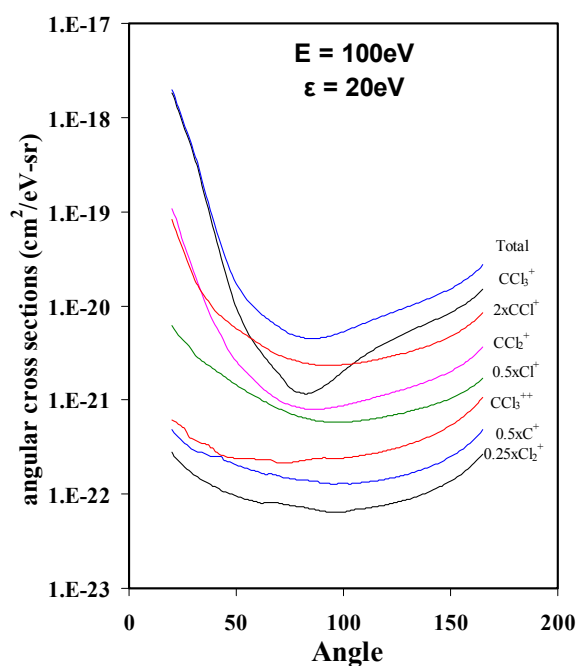
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DETERMINATION OF ANGULAR CROSS SECTIONS FOR ELECTRON DISSOCIATIVE IONIZATION OF CCl₄ MOLECULE

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The CCl₄ molecule has attained a widespread interest in plasma technology and the atmospheric studies. It is used as a reactive etching gas for silicon wafers in semiconductor industry in consequence for plasma modelling study to obliterate the parent molecule. Angle dependent differential cross sections for the product ions CCl_n⁺ (n=0-3), Cl⁺, Cl₂⁺ and CCl₃⁺⁺ resulting from dissociative ionization of CCl₄ by electron collision have been calculated at fixed incident electron energy of 100eV and fixed secondary electron energy of 20 eV. The semiempirical formulation which requires the oscillator strength data as a major input has been employed [1-2]. The results are presented in the figure given below.



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THE FIRST TEST EXPERIMENT PERFORMED AT THE ELECTRON COOLER OF STORAGE RINGS IN LANZHOU

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The cooler storage ring CSR project was launched in 2000 at the Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou. The project consists of two rings, the main cooler storage ring CSRm and the experimental cooler storage ring CSRe. Both CSR rings are equipped with electron cooling devices [1]. In 2007, the installation was completed and the commissioning of CSRs gained great success, a new highly precise generation of collision experiments will become accessible even for the heaviest ion species. The CSR provides unique and unprecedented conditions for experiments based on the use of highly charged ions and in particular for research in the realm of atomic and nuclear physics. The interaction of the brilliant beams of cooled high-Z ions with low-dense gaseous matter as well as with electrons can be now studied under almost completely background free experimental conditions and with highest luminosity [2,3].

Recombination between electrons and ions is one of the most fundamental atomic collision processes for all kinds of plasmas in the universe. For such investigations, the electron cooler of the storage rings can be used as an electron target for ion-electron interaction studies. In the electron cooler environment, two processes compete: dielectronic recombination (DR) and radiative recombination (RR). The rate coefficient, most important parameters in plasma modelling, can be obtained for various electronic configurations and detailed information on the atomic structure can be deduced in addition. Theoretical investigations of the DR process show that DR might be a powerful tool for the investigation of influence of nuclear effects on the atomic structure and may even be used to obtain model independent information on the nuclear structure, e.g. the nuclear charge radius. This has just been confirmed experimentally [4]. Because the experimental storage ring CSRe can accumulate and store radioactive ions produced by nuclear fragmentation, DR experiments open a novel way for studying the ground-state properties of nuclei far from stability.

A commissioning RR experiment was performed at the electron cooler for Ar¹⁸⁺ ions, the results were presently under evaluation. A further RR experiment is being under preparation for krypton ions. A program is planned to be completed before the end of this year for fine detuning the electron beam energy in order to perform high precision DR experiments.

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ANGULAR MOMENTUM TRANSFER AND POLARIZATION DEGREE OF IONS WITH ONE-VALENCE ELECTRON BY ELECTRON-IMPACT

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When velocity distribution of electrons in plasma is anisotropy, ions in excited states have unequal distribution for magnetic sublevels owing to collisions with such electrons. The radiation emitted from ions with unbalanced sublevel population is polarized and its detection is available as a plasma diagnostic tool [1].

The Stokes parameters (P_1 , P_2 and P_3), which are deduced from measurements of the emitted radiation after electron-impact excitation processes, give detailed information about scattering amplitudes for magnetic sublevels [2]. Expectation value of angular momentum component perpendicular to the scattering plane is called *angular momentum transfer* L_{\perp} ($= -P_3$). In electron-atom impact at low energies, the value of L_{\perp} is positive for S \rightarrow P transition at small scattering angles [3]. Srivastava *et al.* [4] reported that L_{\perp} for electron collisions with H-like ions ($Z=2, 6, \infty$) and He-like ions ($Z= 3, 8, \infty$) is also positive at small scattering angles.

Kai *et al.* [5] have found a case where L_{\perp} is negative in low-energy electron scattering with Mg-like Si^{2+} ion using the R -matrix method. We calculate L_{\perp} and polarization degree in electron scattering by Li^{2+} , B^{2+} and Al^{2+} to investigate their behavior for doubly charged ions with one-valence electron systematically. The R -matrix calculation is adopted to obtain transition-matrix for the excitation. Our results show that L_{\perp} in Li^{2+} , B^{2+} and Al^{2+} at small scattering angles is positive, negative and negative, respectively, at low-energies. We will report details of our calculations and results at the HCI conference.

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EFFECTIVE COLLISION STRENGTHS FOR MG-LIKE IRON PEAK IONS

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Berrington et al [1] have calculated effective collision strengths for Fe XV using both the Breit-Pauli and Dirac R-matrix methods. The calculation was undertaken in the spirit of a case study to lay to rest assertions that the Dirac method is superior for such ions. They found good agreement between the two methods. Current development of the DARC program [2] is aimed at improving the quality of the target states. As a first step we have included the Breit interaction directly in the bound-bound continuum hamiltonians. DARC is based on the Dirac-Coulomb hamiltonian and in order to treat heavier systems correctly it is necessary to include the Breit interaction. We have also used Fe XV as a case study for this code development and in addition examined Cr XIII and Ni XVII. The effects on the effective collision strengths for the iron peak ions are as expected small. The work illustrates the extent to which the DARC program can be automated for isoelectronic series.

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Dielectronic and Radiative Recombination of Si to N-like Tungsten Ions

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Dielectronic recombination (DR) is an important recombination process in high temperature plasmas. DR is the resonant electron capture of a free electron, where simultaneously a bound electron of the ions is excited. The resulting doubly excited intermediate state stabilizes by photon emission. Present and future fusion devices are armoured with the heavy element tungsten as wall material which may be sputtered and ionized by the high temperature plasma. The radiative transitions from DR processes contribute to radiation energy loss in fusion plasma, change the charge state balance and satellite lines can alter line shapes, width and intensities of the parent transitions. On the other hand, understanding the radiation pattern of the highly-charged heavy element ions can provide detailed diagnostics of the high-temperature plasma and test atomic structure calculations.

We have performed x-ray spectroscopic measurements of the dielectronic recombination resonance strength for the LMn ($n=3, \dots, 6$) series of Si-like W^{60+} to N-like W^{67+} tungsten ions. Highly charged tungsten ions were produced, stored and excited with the Berlin electron beam ion trap and the emitted radiation was analyzed with a solid state detector. Information on the charge state abundance in the trap was extracted from a fit of the theoretical radiative recombination intensity to measured values. Good agreement was obtained when the fine structure, angular momentum of the recombination channels is taken into account. Our measurement of x-rays from $n=2-3$, $2-4$ and higher DR resonance transitions was compared to relativistic calculations of the DR cross sections and rate coefficients calculated with the Hebrew University Lawrence Livermore Atomic Code (HULLAC). The theoretical predictions for Ne-like tungsten (W^{64+}) [1] were extended with calculations for ions in adjacent charge states and compare well with the observed DR resonance structure.

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Electron Impact Excitation of Ni II

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Considerable demand exists for electron excitation data for the ions of Fe, Co and Ni, since lines from these elements in low ionization stages are observed in many types of astrophysical spectra. Electron scattering from these ions is complicated by the 'open' 3d-shell in the target, which gives rise to hundreds of fine structure levels and thousands of coupled channels. In this study we represent the complex Ni II target by a sophisticated configuration interaction (CI) expansion, based on the following five target configurations - the $3d^9$ ground state configuration and the $3d^84s$, $3d^74s^2$, $3d^84p$ and $3d^74s4p$ excited configurations. These configurations give rise to 295 target states and over 1900 scattering channels if we consider transitions between fine structure levels. We are using the new parallel R -matrix suite of codes (RMATRIXII and PFARM) on HPCx to calculate Maxwellian averaged effective collision strengths for low-lying forbidden transitions in Ni II, over a range of astrophysically significant temperatures. To our knowledge this is the most extensive Ni II R -matrix calculation undertaken to date. Latest results will be presented at the conference. This work is currently supported by a STFC rolling grant.

EFFECT OF ELECTRON-IMPACT IONIZATION IN DAMAGE OF BIO-MOLECULES IRRADIATED BY XFEL

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In x-ray free electron laser (XFEL) application, the analysis of three-dimensional structure of single bio-molecules which almost consist of H, C, N and O atoms is one of the critical issues [1,2]. In this case, target samples are damaged by high-intense x-ray as well as ionization processes by electron impact. The processes are very significant to investigate the damage for electron distribution in the bio-molecule since secondary electrons produced by the high-intense x-ray make the targets ionized again.

There are many reports of ionization-cross section for ground states by electron impact [3]. However, available ionization-cross sections for inner-shell excited states produced by high-intense x-ray have never been reported. In this presentation, we address ionization processes by electron impact for the ground states as well as those for the inner-shell excited states to investigate the damage of the target samples. The cross sections are calculated by using Flexible Atomic Code [4] based on relativistic distorted wave approximation in H, C, N and O atoms and ions.

Figure 1 shows the results of the ionization-cross sections for the ground state in C^{1+} ion. For comparing present result with the recommended experimental result [3], we present the sum of the cross sections for 2s- and 2p-orbital. Our result is good agreement with the recommended data [3]. We compare the results of *L*-shell ionization-cross section for the ground state with those for the inner-shell excited states in figure 2. It is seen that the ionization-cross section for the inner-shell excited states are larger than those for the ground state. We will discuss the effect of electron-impact ionization for the damage to solve rate equation using the present results.

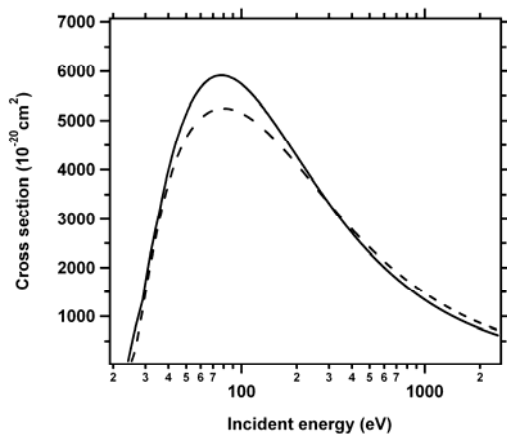


Figure 1 Ionization cross section of C^{1+} . Solid line; present, dashed line; recommended data [3]

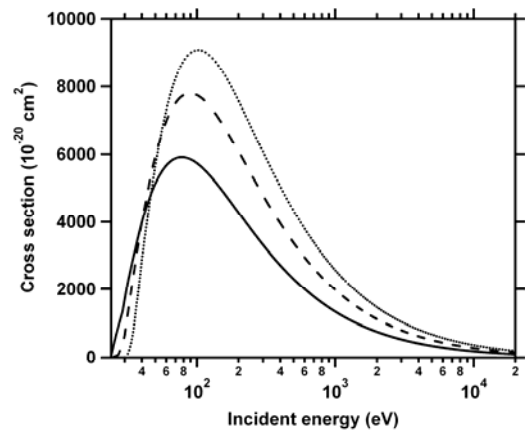


Figure 2 Ionization cross section of C^{1+} . Solid line; $1s^2 2s^2 2p$ state, dashed line; $1s 2s^2 2p^2$ state, dotted line; $2s^2 2p^3$ state.

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HIGH-ENERGY ELECTRON-IMPACT EXCITATION CROSS-SECTIONS OF HYDROGEN-LIKE IRON AND NICKEL IONS

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Electron-impact excitation cross-sections of K-shell ions are used in interpreting the spectra from astrophysical and laboratory produced high-temperature plasmas. Of special importance are K-shell cross-sections of iron and nickel as they have relatively high elemental abundances in celestial sources as well as being present in many laboratory produced high-temperature sources. Yet, for energies well above excitation threshold, where the high-energy tails of the electron temperature-distribution can contribute considerably to the excitation, very little experimental data exist, or none at all.

Here we present a measurement of the cross-sections for the electron-impact excitation of the Lyman- α_1 line of hydrogen-like iron ($Z=26$) and nickel ($Z=28$) over a broad range of energies using the Lawrence Livermore National Laboratory SuperEBIT electron beam ion trap facility. These measurements were performed with electron beam energies between 35 keV and 85 keV. The hydrogen-like spectrum of iron and nickel was observed, and fully resolved, with the NASA/GSFC microcalorimeter which allowed for an absolute cross-section to be measured by normalizing to the radiative recombination x-ray emission. These results are compared to theory.

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ANGULAR MOMENTUM TRANSFER AND POLARIZATION DEGREE OF IONS WITH TWO-VALENCE ELECTRON BY ELECTRON-IMPACT

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The radiation emitted from ions with unbalanced magnetic sublevel population by electron impact is polarized and its detection is available as a plasma diagnostic tool [1]. Kai *et al.* [2] have calculated the polarization degree for He-like ions by electron-impact of the $1s^2\ ^1S_0 \rightarrow 1s2p\ ^1P_1$ transition using the non-relativistic and the semi-relativistic *R*-matrix method.

The Stokes parameters (P_1 , P_2 and P_3) give detailed information about scattering amplitudes for magnetic sublevels [3]. Expectation value of angular momentum component perpendicular to the scattering plane is called *angular momentum transfer* L_{\perp} , and L_{\perp} is equivalent to $-P_3$. In electron-atom impact at low energies, the value of L_{\perp} is positive for $S \rightarrow P$ transition at small scattering angles [4]. Srivastava *et al.* [5] reported that L_{\perp} for electron collisions with H-like ions ($Z=2, 6, \infty$) and He-like ions ($Z=3, 8, \infty$) is also positive at small scattering angles.

Kai *et al.* [6] have found a case where L_{\perp} is negative in low-energy electron scattering with Mg-like Si^{2+} ion using the *R*-matrix method. We calculate L_{\perp} in Be^{2+} and C^{2+} from the ground state to the $2\ ^1P^o$ state by electron-impact to investigate their behavior for doubly charged ions with two-valence electron systematically using the *R*-matrix method. We also calculate the polarization degree for electron-impact excitation of the $3s3p\ ^1P^o$ of Si^{2+} using the same method. Our results show that L_{\perp} in Be^{2+} and C^{2+} at small scattering angles is positive and positive, respectively, at low-energies. We will report details of our calculations and results at the HCI conference.

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ELECTRON IMPACT IONIZATION OF MULTIPLY CHARGED XENON AND TIN IONS

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New interest in electron impact ionization of Xe and Sn ions has been invoked by applications in fusion research and in connection with EUV light sources. Xenon is envisaged as a coolant gas to be injected into the edge plasma of future tokamaks. Further, xenon admixtures in fusion plasmas serve to diagnose a variety of plasma properties including electron temperature and density, as well as ion temperature and impurity transport. In order to predict the effect of xenon injection on the performance of fusion plasmas accurate cross section data are needed. Furthermore, recent interest in applying the EUV radiation of xenon or tin ions to lithography has led to the construction of light sources based on laser-produced plasmas or gas discharges. In the effort to optimize radiation output detailed understanding of the production of the radiating ions is necessary.

We perform absolute measurements of electron-impact single and multiple ionization cross sections for highly charged ions of xenon and tin using an electron-ion crossed-beams technique [1]. Energies range from thresholds to 1 keV. With their many subshells at comparatively low binding energies the xenon ions offer rich opportunities to see processes such as excitation followed by autoionization and resonant electron capture with subsequent multiple electron emission. Because of this reason beside the measurement of absolute cross sections an energy-scanning method is applied to uncover detailed structures in the ionization cross sections which correspond to the population and decay of intermediate excited states. An example for the measurements is shown in Fig. 1.

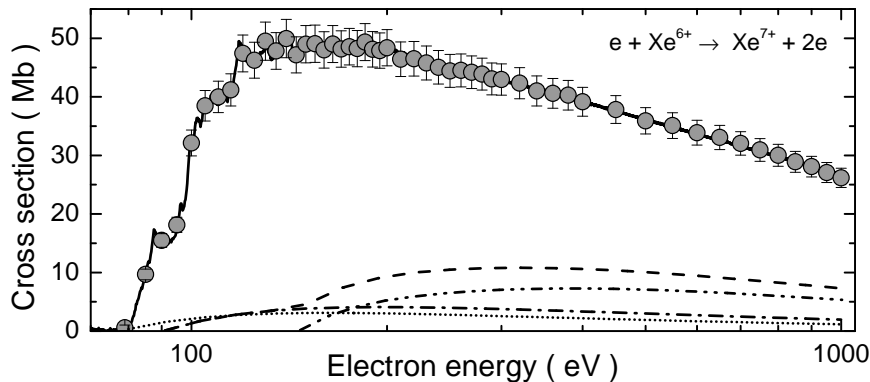


Figure 1: Electron impact ionization cross sections of Xe^{6+} ions: absolute experimental data [shaded circles with error bars]; normalized energy scan [solid curve]; theoretical cross section data for direct ionization of $5s$ [dash-dot] and $4d$ [dash-dot-dot] electrons together with their sum [long-dash curve] calculated by using the LANL atomic physics code package. The dotted curve represents the theoretical cross section of the metastable Xe^{6+} ($5s5p\ ^3P$) configuration assuming a 100% fraction in the incident ion beam.

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EXCITATION RATES FOR TRANSITIONS IN Kr XXXII

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Krypton is an important impurity element in tokamak fusion plasmas where high temperatures ($> 10^6$ K) give rise to many of its ionisation stages. Therefore, atomic data (namely energy levels, oscillator strengths or radiative decay rates, collision strengths, etc.) are required for many ions in order to estimate the power loss from the impurities. In a recent paper [1] we reported energy levels, lifetimes, and radiative rates for four types of transitions, namely electric dipole (E1), electric quadrupole (E2), magnetic dipole (M1), and magnetic quadrupole (M2) for five Kr ions (Kr XXXII - Kr XXVIII). Here we report our results for excitation rates for transitions in boron-like Kr XXXII. These results along with those already reported [1] will be helpful in the modelling of plasmas.

Earlier calculations for Kr XXXII ([2], [3]) included only 20 levels among the $2s^22p$, $2s2p^2$, $2p^3$ and $2s^23\ell$ configurations, reported values of collision strengths (Ω) at a few energies above thresholds, and did not include resonances which can significantly contribute to the determination of excitation rates, even at the high temperatures found in fusion plasmas, at least for some of the transitions. Therefore, in the present work we include 125 levels belonging to the $2s^22p$, $2s2p^2$, $2p^3$, $2s^23\ell$, $2s2p3\ell$ and $2p^23\ell$ configurations of Kr XXXII.

Our calculations are fully relativistic in the jj coupling scheme for which we have adopted the GRASP and DARCF codes. The R -matrix radius is adopted to be 1.48 au, and 15 continuum orbitals are included for each channel angular momentum for the expansion of the wavefunction. This allows us to compute values of Ω up to an energy of 500 Ryd, more than sufficient to determine the values of excitation rates up to a temperature of $10^{7.3}$ K. Furthermore, in order to obtain convergence of Ω for all transitions and at all energies, we have included all partial waves with angular momentum $J \leq 40$. To account for the inclusion of higher neglected partial waves, we have also included a top-up, based on Coulomb-Bethe approximation for allowed transitions and geometric series for others. Resonances in the thresholds region have been resolved in a narrow energy mesh, and results for effective collision strengths (Υ) have been obtained after averaging the values of Ω over a Maxwellian distribution of electron velocities. Detailed results for all 7750 transitions over a wide temperature range below $10^{7.3}$ K will be available during the conference.

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NEUTRON RADIATION EFFECTS ON METAL OXIDE SEMICONDUCTOR (MOS) DEVICES

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The main purpose of this study is to provide the knowledge and data on Deuterium-Tritium (D-T) fusion neutron induced damage in MOS devices. Silicon Metal Oxide Semiconductor (MOS) devices are currently the cornerstone of the modern microelectronics industry. However, when a MOS device is exposed to a flux of energetic radiation or particles, the resulting effects from this radiation can cause several degradation of the device performance and of its operating life. The part of MOS structure (Metal Oxide Semiconductor) most sensitive to neutron radiation is the oxide insulating layer (SiO_2). When ionizing radiation passes through the oxide, the energy deposited creates electron-hole pairs. These electron-hole pairs have been seriously hazardous to the performance of these electronic components. The degradation of the current gain of the dual n -channel depletion mode MOS caused by neutron displacement defects, was measured using *in-situ* method during neutron irradiation. The average degradation of the gain of the current is about 35 mA, and the change in channel current gain increased proportionally with neutron fluence. The total fusion neutron displacement damage was found to be 4.8×10^{-21} dpa per n/cm^2 , while the average fraction of damage in the crystal of silicon was found to be 1.24×10^{-12} . All the MOS devices tested were found to be controllable after neutron irradiation and no permanent damage was caused by neutron fluence irradiation below 10^{10} n/cm^2 . The calculation results shows that (n,α) reaction induced soft-error cross-section about 8.7×10^{-14} cm^2 , and for recoil atoms about 2.9×10^{-15} cm^2 , respectively.

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STRUCTURE DEFORMATION DYNAMICS OF ACETYLENE MOLECULES FOLLOWING ELECTRON LOSS AND CAPTURE COLLISIONS OF 6 MeV O⁴⁺ IONS

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Ion-induced molecular fragmentation has been intensively investigated by using 3D momentum imaging techniques [1-5]. When applied to fragmentation of polyatomic molecules such as CO₂ and C₂H₂, one can obtain important information about structural deformation of a molecule prior to its dissociation because the momentum vectors of product ions are sensitive to the structure prior to dissociation. To date, however the mechanism of structural deformation induced by ion impacts has not been understood yet.

In this work, we investigate the momentum correlation among fragment ions produced by coulomb explosion of acetylene in charge-changing collisions of 6 MeV O⁴⁺ ions. Figure 1 shows an angular correlation between fragment ions of H⁺ and C⁺ produced in (C₂H₂)^{4+***} → (H⁺+C⁺+C²⁺+H) measured for single electron capture collisions. The abscissa θ is the angle between the momenta of two ions $P(C^+)$ and $P(H^+)$. One can see that the spectrum shows two peaks at about 20 and 160 degrees, respectively. This result indicates clearly the two dissociation schemes associated with an intact ion of (C₂H₂)^{4+***}. Namely, they are (HC²⁺-C⁺H⁺) and (H⁺C²⁺-C⁺H) prior to dissociation. In the former case, therefore, both C⁺ and H⁺ move in the same direction after dissociation and separate afterwards as depicted in the figure, giving rise to the correlation angle of 20 degrees. In the latter case, C⁺ and H⁺ start to move in the opposite direction, giving rise to the peak of 160 degrees.

In conclusion, the first stage of molecular dissociation may be understood precisely by the present 3D imaging techniques.

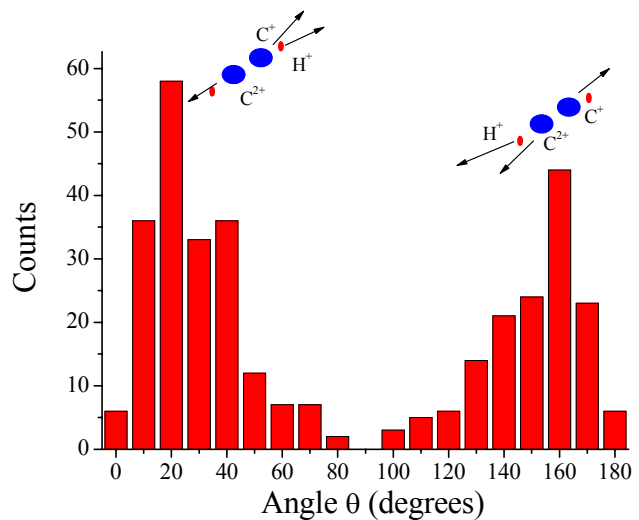


Fig.1 Angular correlation between two momenta of C⁺ and H⁺ produced in (C₂H₂)^{4+***} → (H⁺+C⁺+C²⁺+H) measured for electron capture collisions of 6 MeV O⁴⁺.

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SYSTEMATIC MULTICONFIGURATION DIRAC-FOCK METHOD STUDY OF THE K X-RAY SPECTRA OF SILICON

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Extensive multiconfiguration Dirac-Fock calculations with the inclusion of the transverse Breit interaction and QED corrections [1] have been performed for silicon to explain the influence of removing electrons from L and M shells on the shapes and parameters (the average $K\alpha$ and $K\beta$ transition energies and the values of $K\beta/K\alpha$ intensity ratio) of its K x-ray spectra. For $K\alpha$ and $K\beta$ diagram lines and each types of L - and M -satellite lines the theoretical stick spectra (line positions with their relative intensities) have been presented. Moreover for each type of lines the theoretical spectra being a sum of the Lorentzian natural line shapes [1] have been synthesized.

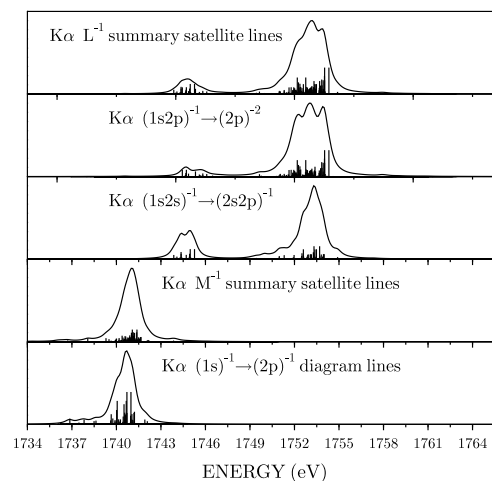


Figure: Theoretical $K\alpha_{1,2}$ x-ray spectra for diagram, L - and M -satellite transitions in silicon.

It has been found that the very large shifts of $K\beta$ and $K\alpha$ transition energies are only in the case of the ionization of the $2p$ and $2s$ subshells. The calculated $K\beta/K\alpha$ intensity ratio is influenced, first of all, by the ratio of the number of electrons in $3p$ and $2p$ subshells, and, secondly, by ionization degree of $2s$ and $3s$ subshells. It is very important to note that the effects of removal of electrons from the subshells on the $K\beta$ and $K\alpha$ transition energies are strong nonadditive, i.e. the $K\beta$ and $K\alpha$ transition energies increase much faster than linearly with the number of holes in a given subshell. Moreover, the effects of removal of electrons from different (L and M) shells on the K x-ray spectra parameters are also strongly nonadditive. The preliminary theoretical results of presented study have been already applied to perform the interpretation of the $K\alpha$ x-ray emission spectra of the low-density SiO_2 aerogel target bombarded by ^{48}Ca ions with initial energy of 11.4 MeV/u measured with a high spectral and spatial resolution along the ion beam stopping path [2]. They can also be helpful in interpreting various silicon target K x-ray spectra induced by photons or different projectiles.

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ELECTRON ANGULAR DISTRIBUTIONS FOR HE SINGLE IONIZATION IN COLLISIONS WITH “FIXED-IN-SPACE” H_2^+ IONS AT 0.5MeV and 1MeV

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Two center effects in collisions of fast ions with H_2 molecules have been intensively studied, both theoretically [1] and experimentally [2]. We investigated in a kinematical complete experiment the ionization He in collisions with H_2^+ -molecular ions at 0.5 and 1MeV at the Max Planck Institute for Nuclear Physics at Heidelberg within a cooperation of Chinese Academy of Sciences and the Max Planck Society. The momenta of the recoiling He ions and the electrons produced in the collisions were measured using a “Reaction Microscope” [3]. The fragments of the H_2^+ were separated by a dipole magnet after the interaction region and detected by two position sensitive MCP detectors. From this information the orientation and internuclear distance of the molecular ion at the instance of the collision could be determined. Pronounced structures are found both in experimental data and theoretical calculations, indicating that the emitted He electron shows a slight preferential emission parallel to the molecular axis. Electron angular distributions in the plane perpendicular to the beam propagation with respect to the molecular axis are shown in Fig.1 and Fig.2 in which case the molecular ion is in the same plane too.

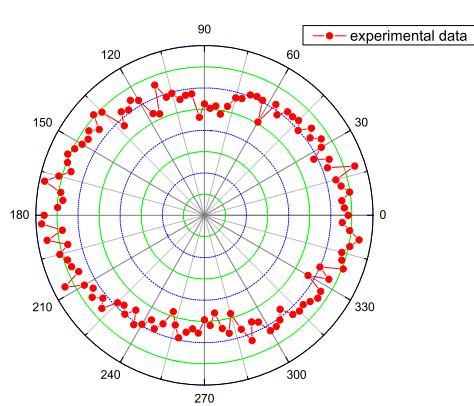


Fig.1 experimental results

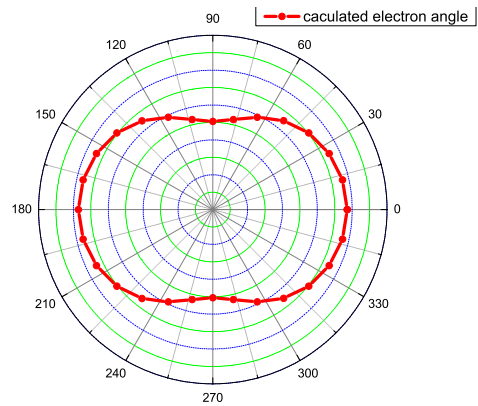


Fig.2 theoretical calculation

Fig.1: Electron emission angle with respect to molecular axis (the molecular axis is along 0 and 180 degree: horizontal line). Fig.2: Theoretical results. Further detailed analysis is under progress.

References

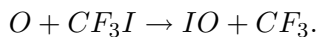
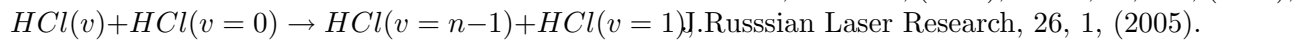
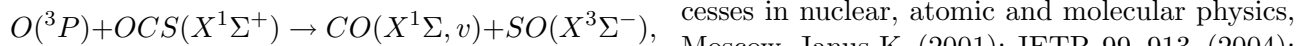
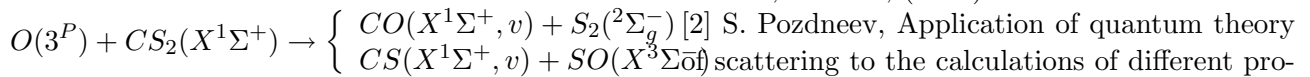
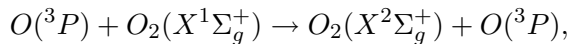
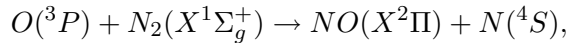
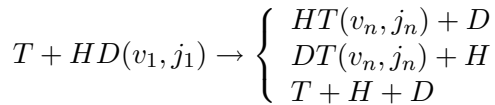
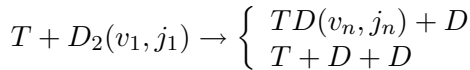
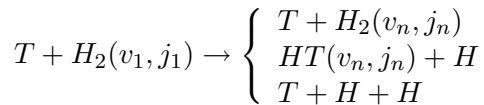
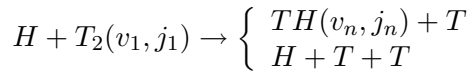
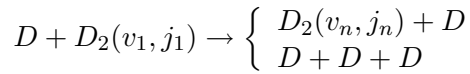
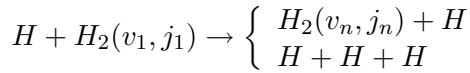
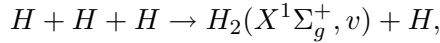
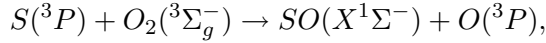
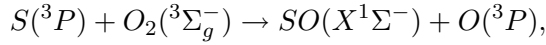
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ELECTRON-MOLECULAR AND ATOM-MOLECULE SCATTERING IN FEW-BODY
APPROACH

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A quantum theory of few-body scattering based on the Faddeev-Yakubovsky equations (FYE)[1] is applied to calculation of the cross-sections of different simplest chemical reactions [2]:



The results of this calculations are compared with available experimental data and of other

approximation. Thus, it is important to understand the physical meaning of numerous approximations applied to the few-body problem and their limitations. The following questions consider in this way. 1. What formalism should be used in investigation of the dynamics of a few-body system? It could be classical or quantum-mechanical equations of the motion, empirical or semi-empirical models, and so on. 2. What is the aim of the simulation? It can be a study of dynamic or static characteristics of a few-body system, calculations of the binding energy, cross sections, rate constants, thermodynamic features, etc. 3. Are the considered models adequate to real physical systems? Answers to many of these questions can be found within the framework of the rigorous mathematical theory suggested by L.D.Faddeev, O.Ya.Yakubovsky and S.P.Merkuriev [1] which describes the dynamics of a few-body system using the correct mathematical basis.

Results of the calculations of the phase shifts, cross sections and Efimov states [1] scattering atom with diatomic molecules based on the three body approximation also are present [2-3].

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BRANCHING RATIO OF N₂ IN COLLISIONS WITH Ar^{q+} ($q \geq 6$) AT ENERGIES BELOW 1 keV/u

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Charge transfer processes involving ionization, electron capture and molecular-fragmentation of multiply charged ions (MCIs) in collisions with atoms and molecules play an important role not only in atomic physics but also in astrophysics and plasma physics. Recently, fragmentation processes of diatomic molecules in electron capture collisions of MCI at energies below 1 keV/u were studied both experimentally[1] and theoretically[2]. In collisions of MCI with diatomic molecules at energies below 1 keV/u, they have experimentally measured two fragment ions in a direction perpendicular to the projectile beam axis in coincidence with the projectile after double and triple electron capture. As a result, an interesting observation of the charge-asymmetry effect between the far and near fragment ions from incident MCI beam axis was reported, i.e., it is dominant process that the far site fragment ion is more highly than near site fragment ion.

In this work, in order to clarify the charge-asymmetry effect, we have measured molecular-fragmentation of N₂ molecule in electron capture collisions of Ar^{q+} ($q \geq 6$) ions in the collision energy from 30 to 150 eV/u and have determined branching ratios for each reaction channel. We used the MCI beam extracted from mini-EBIS (Electron Beam Ion Source). The MCI beam were collided with an effusive target gas of N₂ in a collision region. Outgoing projectile ions from a collision region were analyzed by a parallel plate electrostatic analyzer with a 2D-PSD which resolves energy and scattering angle of the particles. Two fragment ions were detected separately by two time-of-flight analyzers installed respectively at 90° and -90° with respect to the projectile beam axis. All signals were directly recorded by PC through digitizers as a single event.

For the single, double and triple electron capture processes in collisions of Ar^{q+} ($q \geq 6$) ions with N₂ at the collision energies from 30 to 150 eV/u, we have measured the branching ratio of the molecular fragmentation including charge-asymmetry effect. Experimental results involving detailed discussions will be presented at the conference.

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INTERFERENCE EFFECTS IN ELECTRON EMISSION SPECTRA FOR 3 MeV $H^+ + O_2$ COLLISIONS

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In recent studies electron interference effects have been studied for $H^+ + H_2$ [1] and $H^+ + N_2$ [2] collisions. Both primary interference structures analogous to Young's two slit experiment as well as secondary interferences attributed to intramolecular scattering have been observed [1]. The primary interferences observed in 1-5-MeV/u $H^+ + H_2$ collisions [1] showed a strong dependence on the electron observation angle and a smaller dependence on the projectile velocity, while the second-order interferences superimposed on the main oscillatory structures were independent of angle and velocity. More recent results for $H^+ + N_2$ at similar projectile energies revealed apparently only secondary oscillations [2]. In the present work, the experimental investigations are extended to 3-MeV $H^+ + O_2$. As a result of the larger "slit" separation for O_2 of 2.28 a.u., compared with 2.1 a.u. for N_2 and 1.4 a.u. for H_2 , the primary interference structures would be expected to have higher frequencies. Experimental measurements were conducted at Western Michigan University using the tandem Van de Graaff accelerator. A collimated proton beam interacted with an O_2 target supplied by a gas jet. Emitted electrons were detected with a parallel-plate analyzer equipped with a channel electron multiplier for observation angles of 30° , 60° , 90° and 150° with respect to the incident beam direction and for ejected electron energies of 5-400 eV. The measured molecular O_2 cross sections were normalized to corresponding theoretical O_2 cross sections calculated using one-center wave functions. Ratios of the measured experimental to theoretical cross-sections for each angle were fit with a sinusoidal function $f(k) = A[\sin(kcd-w)] + B$ as shown in Fig. 1, where c is a frequency fitting parameter and w allows for a phase shift. Notably, the frequencies of the oscillatory structures are independent of the observation angle while the phase shifts seem to vary systematically with angle, qualitatively in agreement with results for $H^+ + N_2$ [2]. The analysis gives an oscillation interval for O_2 of $\Delta k \sim 4$ a.u., while for N_2 a value of $\Delta k \sim 2$ a.u. was found. The independence of the oscillation frequency on the observation angle suggests the structures are due to secondary interferences with no obvious evidence for primary interferences. However, this conclusion needs further theoretical and experimental investigation.

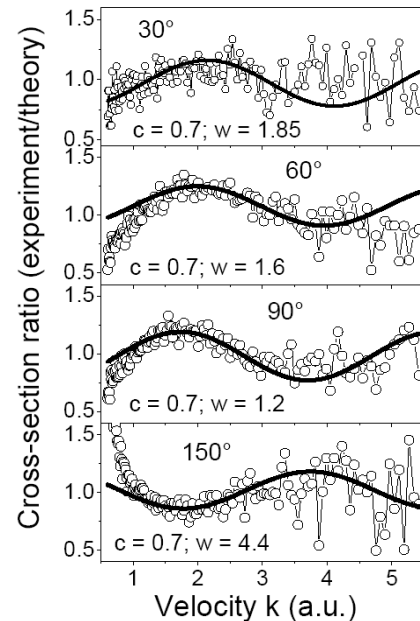


Fig. 1 Experimental to theoretical electron emission cross section ratios for 3 MeV/u $H^+ + O_2$ plotted as a function of ejected electron velocity.

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ELECTRON CAPTURE PROCESSES FROM EXCITED HYDROGEN ATOMS BY HIGHLY CHARGED IONS OF BERYLLIUM AND CARBON

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Until now there have been numerous experimental and theoretical studies for electron capture processes in collisions of highly charged ions with hydrogen atoms being in electronically ground state. However, reports of electron-capture cross sections are scarce for the case of electronically excited hydrogen atoms, in spite of recognitions that such processes are very important for understanding of impurity behavior in tokamak divertors. To our knowledge, only two theoretical estimations have been performed in $C^{4+} + H(n=2)$ collisions, one is classical trajectory Monte Carlo calculation by Zaniol *et al* [1] at a collision energy of 1 eV/amu and the other is molecular state close coupling calculations by Shimakura *et al.* [2].

In this paper, electron-capture cross sections in collisions of bare and Helium-like ions of Be and C with excited H atoms ($n=2$) are calculated in the collision energy range between 60 eV/amu and 6 keV/amu using a molecular state close coupling method.

As an example, the total and partial cross sections for the electron capture into $C^{5+}(nl)$ states in $C^{6+} + H(2s)$ collisions are shown in Fig. 1. This figure shows that electrons tend to be captured into specific state. Furthermore, the cross sections are huge values as anticipated by Macek-Ovchinnikov model [3]. That is to say, the total cross sections in the case of excited hydrogen atoms H(2s) are about twenty times larger compared with that for ground state hydrogen atoms, which is about $40 \times 10^{-16} \text{ cm}^2$ at $E = 1 \text{ keV/amu}$.

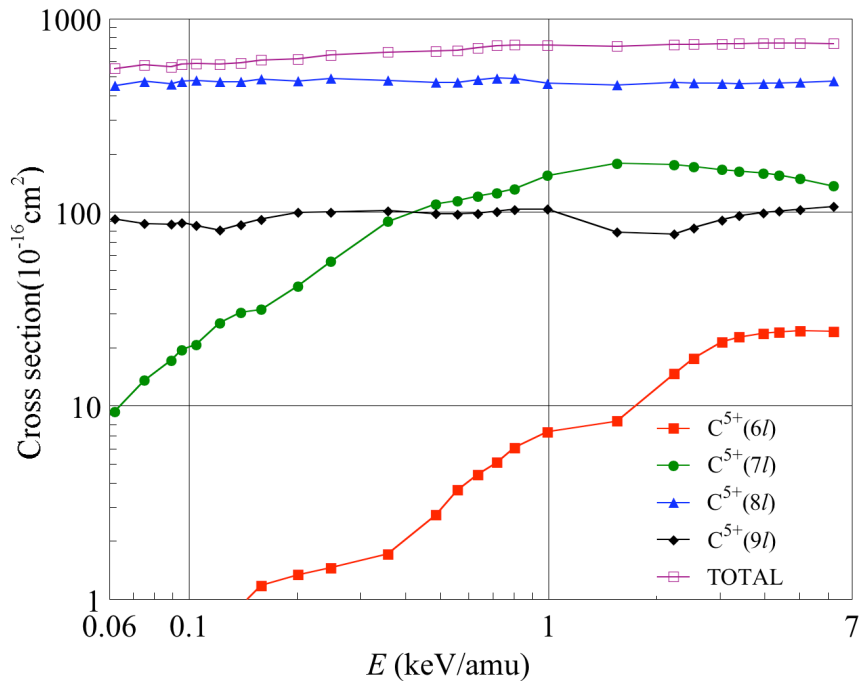


Fig.1 Total and partial cross sections for the electron capture into $C^{5+}(nl)$ states in $C^{6+} + H(2s)$ collisions

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ISOTOPE EFFECT IN DISSOCIATION OF METHANOL DICATIONS PRODUCED BY COLLISION OF Ar^{8+}

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The H/D isotope effects in the dissociation of multiply charged molecular ions stimulate widespread interest since these provide information on the reaction dynamics, for example, intramolecular H migration. So far, strong isotope effects are found for ion-pair dissociation of water dication (HDO^{2+}), that is, the (H^+ , OD^+) channel is much more preferable than the (D^+ , OH^+) channel, and these channels also considerably differ in the kinetic energy release (KER) distributions [1, 2]. In the case of HDO molecule, the D-substitution breaks the C_{2v} symmetry of water, which may be a key factor for strong isotope effects. On the other hand, the isotopomers of methanol may present the isotope effects with keeping the same C_s symmetry. So far, the coincidence study on the dissociation of collisionally prepared methanol dication has been reported [3], whereas the details of the isotope effects in this molecule are still an open question. In the present study, branching ratios and the KER for various ion-pair dissociation channels of methanol dications were measured focusing on the effects of H/D substitution.

The target molecules, methanol and deuterated methanol (CD_3OH and CD_3OD) were doubly ionized by collisions of 120 keV Ar^{8+} , and the fragment ion pairs were detected with using the position-sensitive time-of-flight (TOF) technique. The ion-ion dissociation channels forming $\text{H}^+ \sim \text{D}_3^+$ together with heavier fragment ions as counterparts, two-body dissociation channels and those associated with evaporation of neutral species, were identified in the TOF coincidence map of the fragment ions. The obtained branching ratios do not show notable variation by the H/D substitution.

The KER for each dissociation event was determined from TOFs and positional data. The KER distributions of the two-body dissociation channels yielding trihydrogen cations are shown in Fig. 1, for the three isotopomers. As can be seen in the figure, the KER distributions for the (H_3^+ , CHO^+) and the (D_3^+ , CDO^+) channels are very similar, peaked at about 4.5 eV, whereas that for the (D_3^+ , CHO^+) shifts to the low energy, peaked at about 4.1 eV. It should be noted that the KER distribution of (HD_2^+ , CDO^+) is essentially the same with that of (D_3^+ , CHO^+), that is, the peak position of the sum of these two is also shifted from the other isotopomers. According to double ionization experiments by 30.4 nm photon impact, the peak positions of KER distributions for two-body dissociation channels forming H^+ or D^+ are essentially the same [4]. However in the present study, small differences in the KER distribution for these channels are also observed among isotopomers.

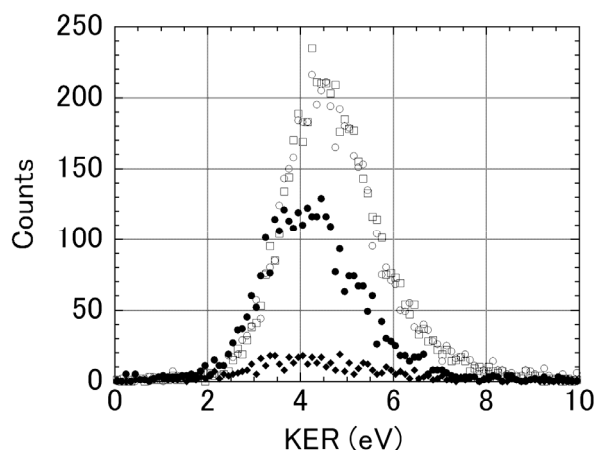


Fig. 1. KER distribution of trihydrogen-forming two-body dissociation channels; ○ (H_3^+ , CHO^+), □ (D_3^+ , CDO^+), ● (D_3^+ , CHO^+), ◆ (HD_2^+ , CDO^+). Since the plots are not normalized by Ar^{8+} beam intensity nor accumulation time, the intensity ratio is meaningful only between the plots ● and ◆.

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ANALYSIS OF CHARGE-ASYMMETRIC COULOMB EXPLOSION OF N₂ MOLECULES WITH SLOW Kr⁸⁺ IONS

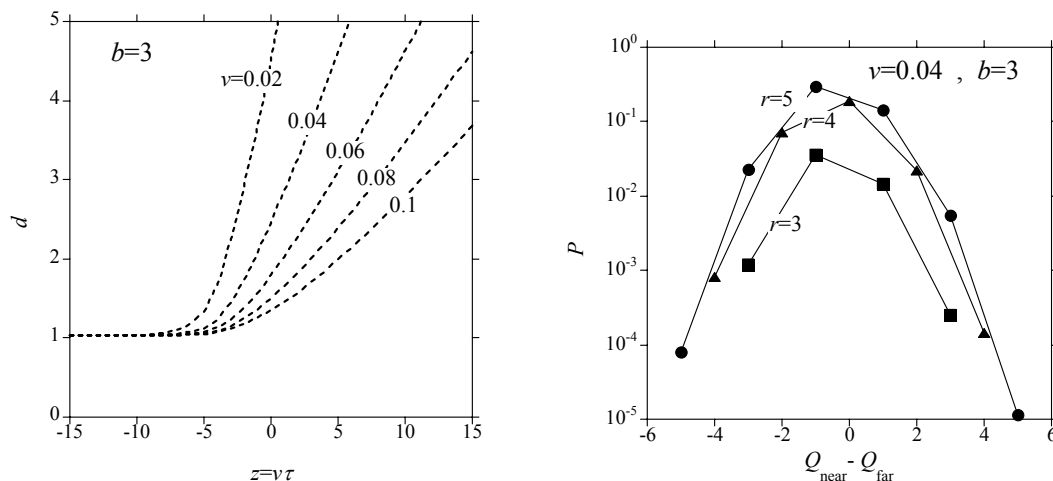
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Much attention has been called to the Coulomb explosion of molecules in a variety of collision processes on the basis of the momentum imaging technique. In particular, Kaneyasu and coworkers [1] have made a triple coincidence measurement in a coplanar geometry for N₂ molecules colliding with slow (10 - 100 eV/amu) Kr⁸⁺ ions. They employ an experimental setup where the fragment ion pair N^{Q+}N^{Q'+} is detected 'back-to-back' transverse to the beam axis and in coincidence with the scattered ion. The most remarkable aspect in their measurement is unequal strengths of charge-asymmetric ($Q \neq Q'$) fragmentation between the near and far sites relative to the point of closest approach on a projectile trajectory [1]. For a given charge pair (Q, Q'), the asymmetry parameter $A = (P_{>} - P_{<}) / (P_{>} + P_{<})$ is obtained through the coincidence populations $P_{>} = P[Q_{\text{far}} > Q_{\text{near}}]$ and $P_{<} = P[Q_{\text{far}} < Q_{\text{near}}]$. The experiment indicates a positive asymmetry $A > 0$; the far site is populated more by the higher charge than by the lower charge.

In this contribution, we analyze the experimental result [1] by taking the three-center Coulombic over-the-barrier model developed by the present authors [2]. We investigate the collisions of Kr⁸⁺+N₂ at velocities of $v = 0.02 \sim 0.1$ atomic unit (*i.e.*, 10 ~ 250 eV/amu) and consider 10 covalent electrons in the N₂ molecule. We assume a linear trajectory of incidence with the impact parameter of $b = 3$, together with a dissociation trajectory retaining the initial orientation. Time evolution $d(\tau)$ of half the bond length is calculated and shown in the left figure, where the horizontal scale is taken $v\tau$, representing the projectile position along the linear trajectory. The probabilities $P(Q_{\text{near}}, Q_{\text{far}}, r)$ are shown in the right figure, where r denotes the number of removal electrons from the molecule. The charge-asymmetry obtained is found consistent with the experimental result [1]. Further calculations for the asymmetry parameter and its velocity dependence are in progress.



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COSTER-KRONIG ELECTRONS FROM N^{q+} ($q=1-3$) RYDBERG STATES PRODUCED IN HIGH ENERGY COLLISIONS WITH He

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In the present, we have measured Coster-Kronig (C-K) electrons from high-Rydberg states produced in 21 MeV(1.5 MeV/u) $N^{3+} + He$ collisions with high resolution to compare with double electron capture (DEC) and dielectronic recombination (DR) processes. We have extended our measurements from N^{3+} to N^{2+} projectile ions. The measured spectra have been compared to our results obtained from 32 MeV(2.0 MeV/u) O^{q+} ($q = 3, 4$) + He [1,2].

For Be-like N^{3+} projectiles, a series of $1s^2 2pnl - 1s^2 2s\ell'$ ($n = 5-9$) C-K transitions is assigned. The high resolution spectrum in the low-energy region, where the $1s^2 2p5l$ state contributes, shows that the line intensity due to the low angular momentum $l = 1$ is the most intense peak, which obeys dipole selection rules. This result for the l distributions is very similar to that for high-energy O^{4+} projectiles, but different from those of the DEC spectrum and also of the DR spectrum where the radiative stabilization is necessary [3].

For B-like N^{2+} projectiles, a series of $1s^2 2s2p(^3P)nl - 1s^2 2s^2\ell'$ ($n = 4-8$) C-K transitions is assigned. In this case, C-K transitions from $1s^2 2s2p(^3P)4l$ states are energetically forbidden for $l = 0$ and 1, but those from the states of $l = 2$ and 3 are clearly observed. For the higher n , the angular momenta of $l = 0-3$ states are populated. The measured spectra have been compared with dielectronic recombination (DR) processes [4].

We have also measured Coster-Kronig electrons from high-Rydberg states produced in 14 MeV(1.0 MeV/u) $N^+ + He$ collisions. For C-like N^+ projectiles, the C-K electron spectra are more complicated than those from Be-like N^{3+} and B-like N^{2+} projectiles. A series of $1s^2 2s2p^2(^4P)nl - 1s^2 2s^2 2p\ell'$ ($n = 3-8$) C-K transitions is clearly assigned. A detailed analysis will be presented at the conference.

Autoionization has been systematically observed from high Rydberg states in N^{q+} ($q = 1-3$) ions for the first time, which are created by the electron excitation in N^{q+} projectile ions in collisions with He.

This work is supported by the Common Use Program of JAEA.

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COSTER-KRONIG ELECTRONS FROM O^{q+} ($q=1-4$) RYDBERG STATES PRODUCED IN HIGH ENERGY COLLISIONS WITH He

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Recently we have reported on Coster-Kronig (C-K) electron spectra in high energy collisions of 32 MeV O^{4+} and O^{3+} ions with a He gas target [1,2]. For Be-like O^{4+} projectile ions, the C-K spectra are compared with double electron capture (DEC) [3-5]. For B-like O^{3+} ions, we compared with previous results [6] and confirmed the autoionization transition from the $1s^2 2s 2p(^3P) 5s$ state. In the present, we have measured systematically C-K electrons from high-Rydberg states produced in high energy collisions of 30 MeV O^{2+} and 15 MeV O^+ ions with a He gas target and also of 32 MeV $O^{3+,4+}$ ions with higher resolution.

For Be-like O^{4+} projectiles, a series of $1s^2 2p(^2P) nl - 1s^2 2s \ell'$ ($n = 6-11$) C-K transitions is assigned. The high resolution spectrum for the $1s^2 2p 6l$ state shows that the line intensity due to the low angular momentum $l = 1$ is the most intense peak, which obeys dipole selection rules. This result for the l distributions is found to be different from those of the DEC [3-5]. For B-like O^{3+} projectiles, a series of $1s^2 2s 2p(^3P) nl - 1s^2 2s^2 \ell'$ ($n = 5-11$) C-K transitions is assigned. It is found that the angular momenta of $l = 0-3$ states are populated and the maximum intensity is attributed to the states with higher angular momenta $l > 1$. the C-K spectra are also compared with dielectronic recombination (DR) processes [7].

For C-like O^{2+} projectiles, a series of $1s^2 2s 2p^2(^4P) nl - 1s^2 2s^2 2p \ell'$ ($n = 4-9$) C-K transitions is clearly assigned. This means that these transitions are mainly due to $2s-nl$ electron transition of the ground state $O^{2+} 1s^2 2s^2 2p^2(^3P)$ to the $1s^2 2s 2p^2(^4P) nl$ excited state. For N-like O^+ projectile ions, the C-K electron spectra are much more complicated than those from the other charge states of ions, i.e., Be-, B- and C-like $O^{4+,3+,2+}$ ions. A detailed analysis of ejected electron spectra for these collision systems is still underway and will be presented at the conference.

This work is supported by the Common Use Program of JAEA.

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SINGLE CHARGE TRANSFER IN COLLISIONS OF DIATOMIC MOLECULES WITH SLOW HIGHLY CHARGED IONS

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An analytic study is presented of asymptotic properties of the three-center quasimolecular system $A_2^{(Z_a-1)+} + B^{Z_b+}$ consisting of a homonuclear diatomic molecule $A_2^{(Z_a-1)+}$ and a highly charged atomic ion B^{Z_b+} . The potential of the one-electron exchange interaction of this system is calculated asymptotically correctly (for large distances R between interacting particles) in the framework of the non-perturbative semiclassical and the Landau-Herring approaches. The total cross sections of the electron capture in $H_2 + Ar^{q+}$ ($q = 6, 8, 14, 16$) collisions in the energy region from 5.0 to 2×10^3 eV/amu were calculated and compared with available experimental and theoretical data (see Fig. 1). It is shown that with increasing of projectile (atomic ion Ar^{q+}) charge, use of the semiclassical expression describing such electron exchange interaction provides noticeably better (than with use of the Landau-Herring one) agreement between the calculated cross sections and experimental data.

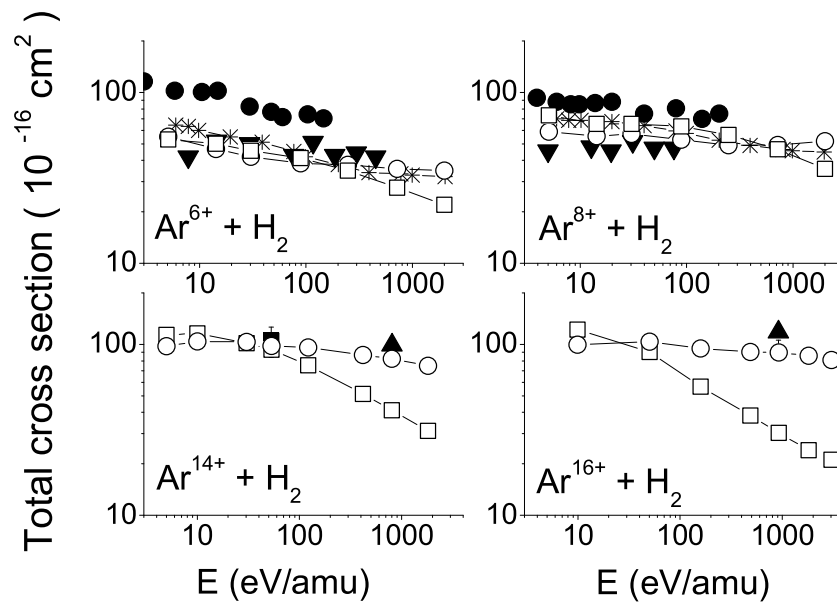


Figure 1: The total cross sections for single electron capture in $H_2 + Ar^{q+}$ ($q = 6, 8, 14, 16$) collision. Theory, —*— : MO-calculation from Ref. [1a]. Present calculations, —○—: semiclassical approach; —□—: Landau-Herring approach. Experimental data, ●: Ref. [1a]; ▼: Ref. [1b]; ▲: Ref. [2a], ■: Ref. [2b].

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THEORETICAL PREDICTIONS OF THE STRUCTURE OF M-X-RAY LINES OF HEAVY ATOMS

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A very complex origin of the X-ray spectra of target atoms, resulting from multiple ionization, makes it absolutely essential to carry out theoretical study on the effect of the ionization of various shells on the positions and shapes of different K -, L - and M -X-ray lines [1-3]. In the present work very extensive multiconfiguration Dirac-Fock calculations with the inclusion of the transverse (Breit) interaction and QED corrections have been carried out on gold, thorium and uranium to elucidate the structure of various satellite (additional vacancies in N and/or O shells) and hypersatellite (additional vacancies in M or M and N shells) $M\alpha_{1,2}$ ($M_5N_{6,7}$) and $M\beta_1$ (M_4N_6) lines in its X-ray spectra. For every calculated type of $M\alpha_{1,2}$ and $M\beta_1$ lines the theoretical stick spectra (line positions with their relative intensities) have been presented. Moreover for each type of lines two theoretical spectra have been predicted: one being a sum of the Lorentzian natural line shapes and the other one being a convolution of the sum of the Lorentzian natural line shapes with the Gaussian instrumental response. The obtained theoretical results will be very helpful in reliable and quantitative interpretation of a very complex origin structure of $M\alpha_{1,2}$ and $M\beta_1$ lines in various high-resolution X-ray spectra of heavy atoms induced by different light and heavy projectiles.

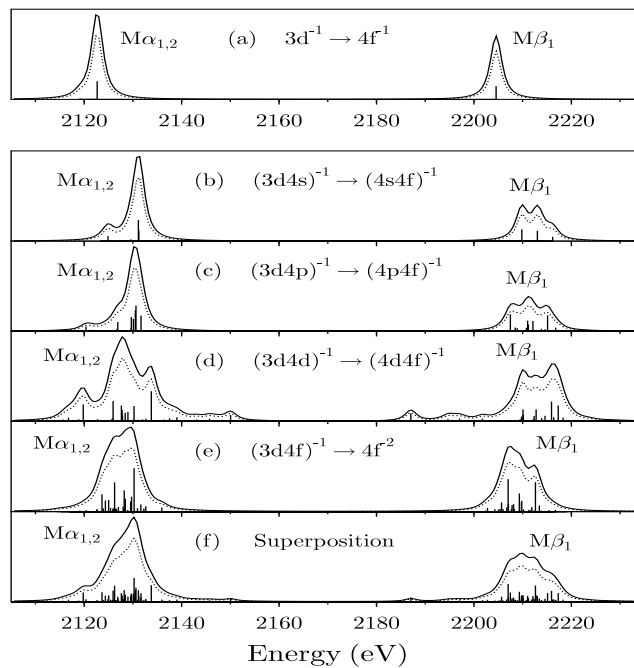


Figure 1: Calculated stick and predicted spectra for the $M\alpha_{1,2}$ and $M\beta_1$ diagram [spectrum (a)] and N-shell satellite transitions [(b)-(f)] in gold. Spectrum (f) is the summary spectrum [(b)+(c)+(d)+(e)].

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INFLUENCE OF CHANGES IN THE VALENCE ELECTRONIC CONFIGURATION ON THE STRUCTURE OF L-X-RAY SPECTRA OF MOLYBDENUM

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The $L\alpha_{1,2}$ ($L_3M_{4,5}$) and $L\beta_1$ (L_2M_4) lines in the X-ray spectra of molybdenum induced by X-ray photons, 279-MeV oxygen ion and 178-MeV neon ion beams [1] have been measured by means of a high-resolution von Hamos crystal spectrometer having the energy resolution of about 1 eV. In the present work extensive multiconfiguration Dirac-Fock calculations with the inclusion of the transverse (Breit) interaction and QED corrections [2] have been carried out on molybdenum to explain the dependence of the structure of $L\alpha_{1,2}$ and $L\beta_1$ lines on the changes in configurations of the valence electrons [belonging to a different of the three $4d^{m-r}5s^r$ ($r=2,1,0$) types]. The most complicated case occurs for the $4d^55s^1$ configuration (see Figure 1), in which occupation of $4d$ shell and $5s$ shell is half-and-half. For this case we have 417 initial states of the type $2p^{-1}$, 647 final states of the type $3d^{-1}$, and 119 383 X-ray transitions. The obtained results are very helpful in reliable and quantitative interpretation of a very complex origin structure of $L\alpha_{1,2}$ and $L\beta_1$ lines in various high-resolution X-ray spectra of $4d$ transition-metals induced by X-ray photons and different light and heavy projectiles.

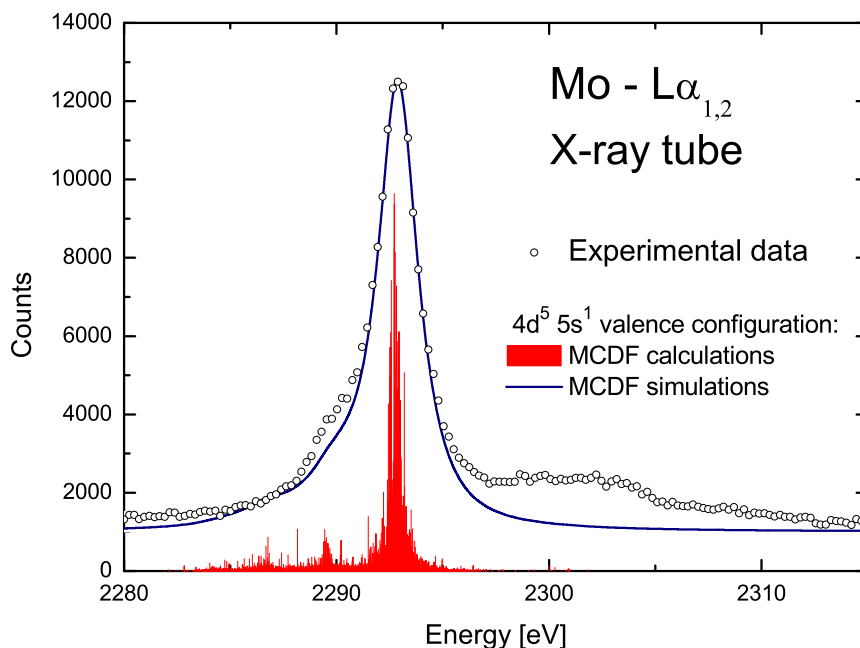


Figure 1: Comparison of the measured structure of the X-ray spectrum of molybdenum induced by X-ray photons with the MCDF predictions for diagram $L\alpha_{1,2}$ lines in the case of $4d^55s^1$ configuration.

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CHARGE TRANSFER CROSS SECTIONS OF W^{2+} IONS IN COLLISIONS WITH RARE GAS TARGETS

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Charge transfer is one of the important collision processes not only for atomic physics but also for controlled thermonuclear fusion. The understanding of charge transfer processes is essential for studying the influence of impurity ions in fusion plasma. From this point of view, Itoh *et al.* and Imai *et al.* have measured charge transfer cross sections of Be, B, C, Cr, Fe, and Ni ions in collisions with He, Ne, Ar, Kr, H₂, CO, CO₂, CH₄, C₂H₆, C₃H₈, CO, CO₂ and N₂ targets at energies less than a few keV/u [1,2]. Recently, higher-Z elements including tungsten have been proposed as the divertor plate material of the ITER (formerly, International Thermonuclear Experimental Reactor). As experimental and theoretical investigations of charge transfer for tungsten ions are still scarce now, we have started experimental study of charge-transfer cross sections for highly charged tungsten ions colliding with atomic and molecular gas targets.

Figure schematically shows the present experimental setup. The experiment has been done using the Van de Graaff Accelerator Facility of the Quantum Science and Engineering Center, Kyoto University. Doubly charged tungsten ions are obtained by Ion-Impact-Ion-Source. A beam of 0.8-MeV CO₂⁺ ions from the accelerator were focused on a pure tungsten wire set in a sputter-type ion source. Sputtered ions were extracted perpendicularly to the CO₂⁺-beam direction, and were accelerated to the desired kinetic energy.

The extracted ions were then focused by an einzel lens, and were momentum-analyzed by a Wien-filter. Neutrals produced in collisions with residual gases through beam passage were rejected electrostatically by a neutral particle rejector. The analyzed W^{2+} ion beam was impinged upon gas target in a collision cell. Outgoing ions were electrostatically deflected according to their charge states, and were detected by a position-sensitive MCP detector with a resistive anode.

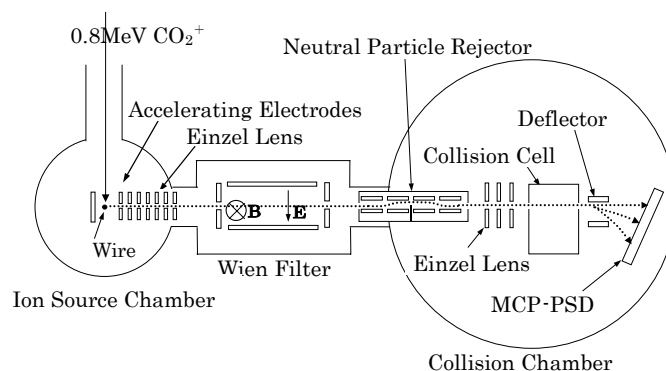


Figure Experimental setup.

Measurements for $W^{2+} + \text{Ne, Ar, Kr}$ collisions at 15 keV have been in progress. The obtained data will be compared with the previous data for other high-Z ions [2], and discussed at the conference.

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X-RAY SIGNATURES OF CHARGE EXCHANGE IN L-SHELL IONS

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The X-ray signature of L-shell charge exchange in Sulfur was studied in the laboratory. Charge states from S^{11+} to S^{14+} were created in the LLNL Electron Beam Ion Trap and were left to interact via charge exchange with neutral SF_6 gas. The measurements were monitored with the EBIT Calorimeter Spectrometer. Comparison of these charge exchange (CX) spectra with those obtained under electron-impact excitation showed marked differences. In the CX spectra, an enhancement was observed in the high- n transitions; $n = 4, 5, 6 \rightarrow n = 2$, in comparison to the $n = 3 \rightarrow n = 2$ transitions that dominate the direct excitation spectra. An even greater enhancement was recorded in transitions from the levels of electron capture to the ground states; $n_c = 7, 8, 9 \rightarrow n = 2$. The spectra mainly consist of S^{13+} lines, but lower charge states such as S^{12+} , S^{11+} and S^{10+} are also present. These are the first high-resolution results of L-shell charge exchange. The spectra have been compared to low-resolution data on charge exchange in L-shell Iron, and showed a similar spectral structure. However, the high-resolution spectra from Sulfur exhibit a significant enhancement in transitions from the electron capture-levels $n_c=7, 8, 9$, whereas the low-resolution spectra of Iron showed the greatest enhancement in the transitions from $n=4, 5$ levels.

Part of this work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and NASA grants to LLNL, SAO, and GSFC.

STUDIES OF X-RAY PRODUCTION FOLLOWING CHARGE EXCHANGE RECOMBINATION BETWEEN HIGHLY CHARGED IONS AND NEUTRAL ATOMS AND MOLECULES

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We have used microcalorimeters built by the NASA/Goddard Space Flight Center and the LLNL EBIT facility to measure x-ray emission produced by charge exchange reactions between highly charged ions colliding with neutral helium, hydrogen, and nitrogen gas. Our results show the measured spectral signatures produced by helium, hydrogen, and nitrogen donors. The measurements are compared to theory where available. These results can be used to interpret x-ray spectra produced by a variety of laboratory and celestial sources including cometary and planetary atmospheres, the Earth's magnetosheath, the heliosphere, tokamaks, and electron beam ion traps.

Part of this work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and is also supported by NASA grants to LLNL, SAO, and the NASA/GSFC.

VACUUM ULTRAVIOLET SPECTRA IN CHARGE TRANSFER COLLISIONS OF MULTIPLY CHARGED Sn IONS

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The Mo/Si multilayer mirrors having peak reflectivity around 13.5 nm, which is in the extreme ultraviolet (EUV) region, will be used in the next-generation semiconductor lithography. The laser-produced Sn plasma, which has strong emission around 13.5 nm, is a promising light source for the EUV lithography. However, there is not enough spectroscopic information about multiply charged Sn ions composing Sn plasmas. In order to provide the spectroscopic data of multiply charged Sn ions, we have measured the EUV emission spectra following charge transfer collisions of the charge-selected Sn ions with neutral gas targets. The experimental results on the unresolved transition array (UTA) have been employed in the hydrodynamical simulation of the Sn plasma [1].

Not only the “in-band” light around 13.5 nm, but also the “out-of-band” light with wavelengths longer than 130 nm can be reflected by the Mo/Si mirror in the EUV exposure system with high reflectivity. In this work, we measured the VUV (vacuum ultraviolet) emission spectra by means of charge exchange spectroscopy. Figure 1 shows the emission spectra in collisions of Sn^{q+} ($q = 3 - 6$) with Xe measured with a compact Seya-Namioka spectrometer. As can be seen in this figure, several lines have been observed in collisions of different charge ions. This finding means that the multiple-electron capture processes are significant in these collisions. Generally, the single-electron capture is dominant in collisions of highly charged ions, and the scaling law can be applied for the capture cross sections. However, the double-electron capture can be significant in collision of moderately charged ions [2].

Some of the emission lines observed in collisions of $q \leq 5$ ions are assigned by literature, and others could be done by using the established energy levels. However, several lines in collisions of $q = 6$ can not be identified because of no information. We have performed the similar measurements using the other rare gas targets. The emission spectra strongly depend on the target gases.

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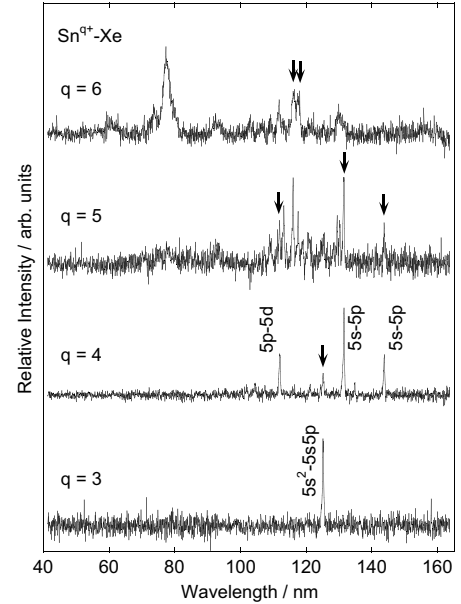


Figure 1: The emission spectra in collisions of Sn^{q+} ($q = 3 - 6$) with Xe. The lines indicated by arrows are considered to be emissions from ions which are produced by the double-electron capture.

DISSOCIATIVE AND NON-DISSOCIATIVE CHARGE-CHANGING PROCESSES IN 1.0-2.0 MeV/u $O^{5+} + O_2$ COLLISIONS

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Fundamental interactions of molecular oxygen in collisions with charged particles are relevant to many fields of study including astrophysics, atmospheric physics, and the life sciences. In an effort to gain additional understanding of such interactions, dissociative and non-dissociative products of O_2 associated with single electron capture, single electron loss, and direct ionization have been measured for 1.0, 1.5, and 2.0 MeV/u $O^{5+} + O_2$ collisions. These measurements were conducted at Western Michigan University using the tandem Van de Graaff accelerator. Time-of-flight techniques were used to detect coincidences between target ion fragments and individual outgoing projectile charge state components. A collimated O^{5+} beam interacted with O_2 contained within a differentially pumped target gas cell, in which the pressure was kept below 2.0 mTorr. Recoiling target ions were extracted by an electric field transverse to the beam direction and detected with a set of coupled microchannel plates. Following interaction with the target gas, the projectile beam was magnetically analyzed and the individual charge-changed components were counted using silicon surface-barrier detectors. To ensure the validity of the data, spectra for He [1] and Ne [2] were collected and the ratios for multiple ionization were compared with previously measured values as well as the measured yields for total single electron capture and loss [1]. These latter yields also provided the calibration factor to determine absolute cross sections for the O_2 data. In all cases, spectra were measured for several target pressures to check for single-collision conditions. Fig. 1 shows the target ion products associated with projectile electron capture in 1.0 – 2.0 MeV/u $O^{5+} + O_2$ collisions compared with the corresponding spectrum for 2 MeV/u $O^{5+} + Ne$. Both non-dissociative molecular and dissociative atomic products are formed with charge states up to 4+. In Fig. 1 the total integrated beam current is the same for each spectrum, indicating a strong decrease in the relative cross sections as a function of projectile energy. The spectra for projectile electron loss and direct ionization gave similar results. Absolute cross sections will be calculated, as well as the relative yields for dissociative and non-dissociative ionization of O_2 to determine detailed information on the mechanisms for the molecular fragmentation of O_2 . Additional measurements for incident oxygen charge states 6, 7, and 8+ will be carried out to determine the charge-state dependence of the various processes.

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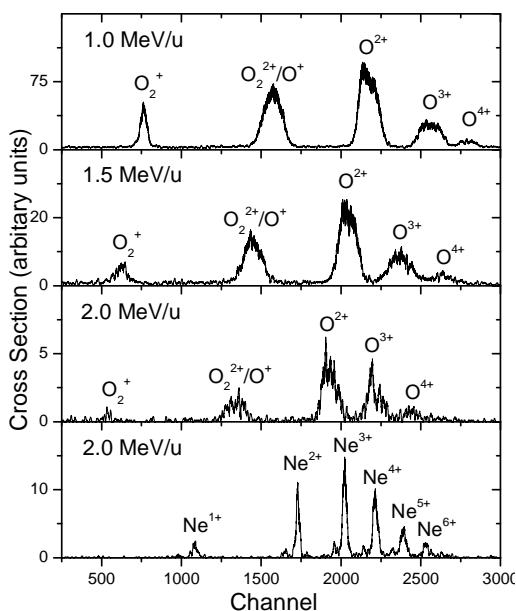


Fig. 1 Target ion fragments associated with projectile electron capture for 1.0, 1.5, and 2.0 MeV/u $O^{5+} + O_2$ collisions compared with the corresponding spectrum for 2.0 MeV/u $O^{5+} + Ne$.

CHARGE TRANSFER PROCESSES IN COLLISIONS OF SLOW HIGHLY CHARGED IONS WITH POLAR MOLECULES CO AND C₃H₈

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Charge transfer processes resulting from low energy collisions of polar molecules CO and C₃H₈ with highly charged Be²⁺ and B²⁺ ions have been investigated experimentally and theoretically. The experiment was performed using the Van de Graaff Accelerator Facility of the Quantum Science and Engineering Center, Kyoto University. A schematic view of the experimental apparatus is given in Fig. 1a. Theoretical study based on a semiclassical analysis of the wave function of tunneling electron (see Ref. [1]) was also carried out. The potential for the one-electron exchange interaction between a non-central target (polar molecule) and projectile (atomic ion) were obtained in closed analytical form. Our theoretical calculations for absolute cross sections of the electron transfer have been found to be in fairly good agreement with the measured data (see Fig. 1b).

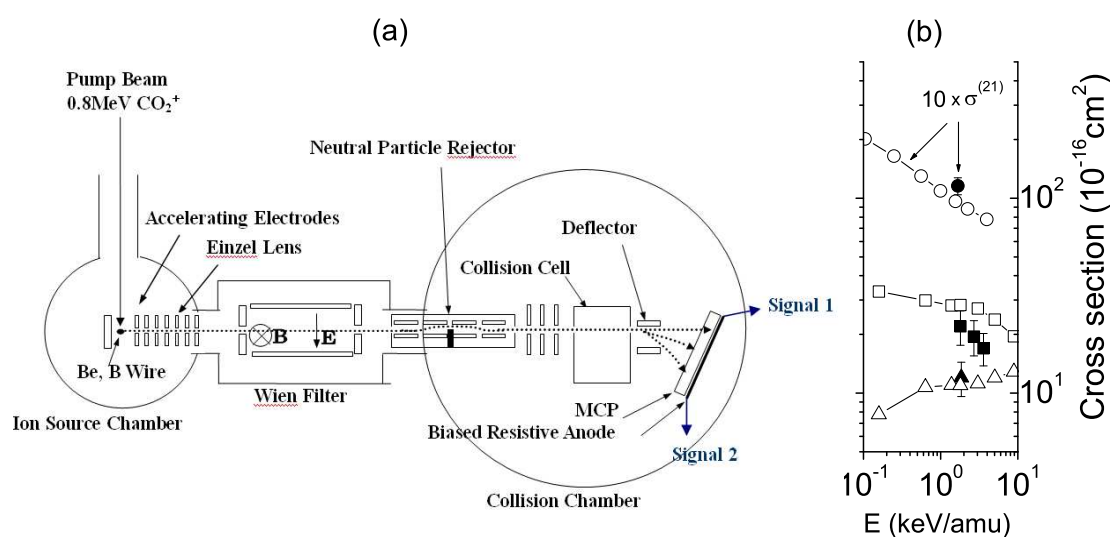


Figure 1: (a). The experimental setup. (b). Measured cross sections for single electron capture $\sigma^{(21)}$, \blacksquare : C₃H₈ + Be²⁺; \bullet : CO + Be²⁺; \blacktriangle : CO + B²⁺. Solid lines with open symbols: present calculations. [In this figure cross sections for the collision CO + Be²⁺ multiplied by a factor of 10].

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SINGLE ELECTRON CAPTURE IN COLLISIONS OF N^{2+} WITH He AT LOW ENERGIES

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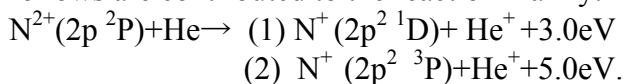
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The absolute total cross sections for single electron capture of N^{2+} on He have been measured in the energy range between 0.1 and 300 eV/u. In the collision system, the differential cross sections for single electron capture have an enlargement at 0 degree, which may be responsible for the glory scattering [1]. In slow neutral-neutral collisions, it is well known that an oscillatory structure due to glory effect may appear on the total cross sections [2]. In ion-atom collisions, there is no report about the oscillatory structure. We confirmed whether the oscillation can be observed or not even for ion-atom collisions to measure the fine energy dependence of the cross sections.

The apparatus and the experimental procedure used in this study have already been described elsewhere [3]. Only the brief features are summarized here. The apparatus consists of a tandem mass spectrometer and an EBIS type ion source. The collision cell in the spectrometer possess ion beam guide system named Octa Pole Ion beam Guide (OPIG) which prevent slow ion beam from diverging with RF field. Using the OPIG, we can decrease the collision energy down to 0.1 eV/u. The absolute gas pressure was measured with MKS Baratron type 690A. The energy width of the primary ions is estimated about $\Delta E=0.2$ eV/u.

The cross sections measured are shown in figure 1. The energy dependence of the cross sections has interesting structures. In the collision energy below 1eV/u, the cross sections have a little scattering tendency. And around the collision energy of 70 eV/u, a clear dip can be observed on the cross sections.

In low energy region, the two paths as follows are contributed to the reaction mainly:



The grand state of quasi-molecular potential corresponding to the reaction path of (2) has a potential well with 2 eV [4]. The attractive potential surface is considered the cause of the glory scattering. Though the clear evidence of the oscillation could not be observed on the cross sections, the scattering tendency in low energy region may be responsible for the glory effect. The reason of appearance of the dip is considered that the main path is changed from (2) to (1) with increasing the collision energy.

In the present measurements, it is known that the precise measurement of energy dependence of total cross sections can be access the information of reaction potential energy surface.

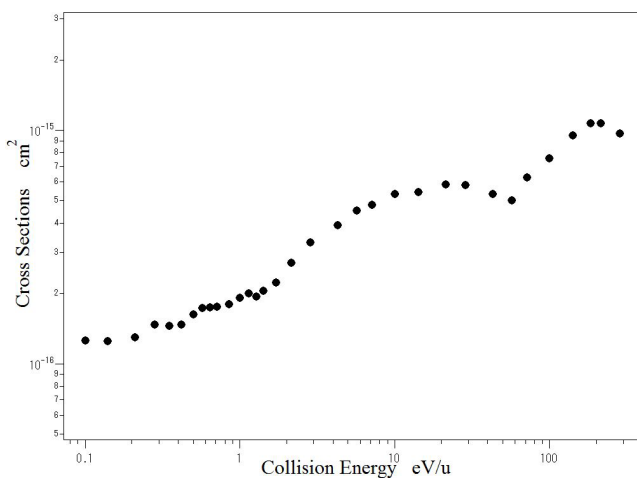


Figure 1. Present single electron capture cross sections in collisions of N^{2+} with He.

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GROSS AND PARTIAL IONIZATION CROSS SECTIONS IN 6-MEV/AMU BARE-ION COLLISIONS WITH METHANE

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For understanding the ionization mechanisms in molecules, gross ionization cross sections have been measured with a condenser-plate method in bare ion impact on CH₄ molecules. Moreover, a mass-spectroscopic technique has been applied to separate recoiled ions to get partial ionization cross sections. Secondary ions produced in collisions were extracted with an electrostatic lens, mass/charge-analyzed by a double focusing sector magnet and finally detected by a Channeltron detector. The projectile ions such as 6-MeV/amu-H⁺, -He²⁺, -C⁶⁺, -Ne¹⁰⁺ and -Ar¹⁸⁺ were provided by the Heavy Ion Medical Accelerator in Chiba (HIMAC) of the National Institute of Radiological Sciences.

In Fig. 1, mass/charge spectra for CH₄ in H⁺ and Ne¹⁰⁺ impact are shown for comparison. They are characterized by several peaks corresponding to fragmented ions as well as the most prominent peak for parent CH₄⁺ ions. It can be noted that relative intensities of the fragmented ions increase as the projectile charge increases.

Partial ionization cross sections can be calculated from the relative intensities of the peaks in mass spectra and gross ionization cross sections measured in a separate experiment. Figure 2 shows the obtained partial cross sections as a function of projectile charge q . The cross sections for CH₄⁺ and CH₃⁺ ions are prominent, and they increase with a slope of around 2 in a log-log plot. This indicates that they are mainly produced at distant collisions, where the first Born approximation would be applicable. On the other hand, fragmented ions, such as CH₂⁺, CH⁺ and C⁺, show charge dependence quite different from the Born approximation, indicating that other mechanisms might contribute to their production. Doubly and triply charged carbon ions have been detected with remarkable intensities in highly charged Ne¹⁰⁺ and Ar¹⁸⁺ ion impact.

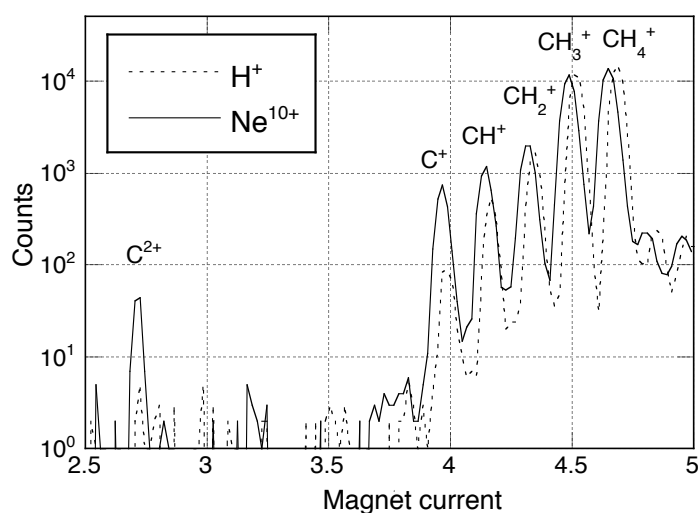


Fig. 1

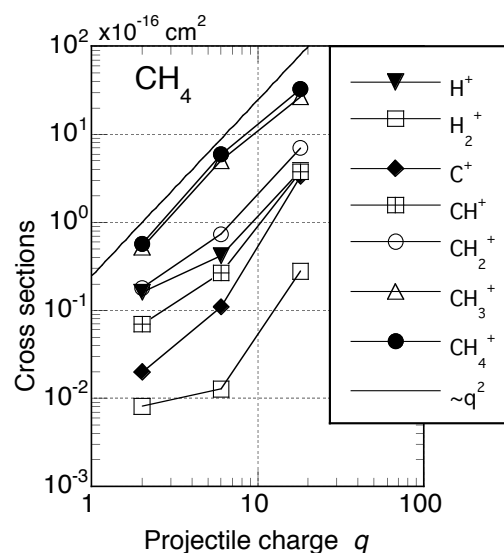


Fig. 2

QED APPROACH TO CALCULATING ELECTRON COLLISION STRENGTHS FOR MULTICHARGED IONS IN A PLASMA: WITHIN THE DEBAE APPROXIMATION

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We present the uniform energy approach, formally based on the QED perturbation theory (PT) [1,2] for the calculation of electron collision strengths and rate coefficients in a multicharged ions (in a collisionally pumped plasma). An account for the plasma medium influence is carried out within a Debae shielding approach. The aim is to study, in a uniform manner, elementary processes responsible for emission-line formation in a plasma. The electron collision excitation cross-sections and rate coefficients for some plasma Ne-like multicharged ions are calculated within QED energy approach [1,2]. The energy shift due to the collision is arisen at first in the second PT order in the form of integral on the scattered electron energy ϵ_{sc} :

$$\text{Im}\Delta E = \pi G(\epsilon_{iv}, \epsilon_{ie}, \epsilon_{in}, \epsilon_{sc})$$

where G is the squared combination of the two-particle matrix elements:

$$V(1,2;4,3) = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)}(-1)^{j_1+j_2+j_3+j_4+m_1+m_2} \times \\ \times \sum_{\lambda, \mu} (-1)^\mu \begin{bmatrix} j_1 \dots j_3 \dots \lambda \\ m_1 \dots m_3 \dots \mu \end{bmatrix} \begin{bmatrix} j_2 \dots j_4 \dots \lambda \\ m_2 \dots m_4 \dots \mu \end{bmatrix} (Q_\lambda^{Qul} + Q_\lambda^{Br})$$

The values Q_λ^{Qul} , Q_λ^{Br} are corresponding to the the Coulomb part $\exp(i\alpha r_{12})/r_{12}$ and Breiht part $\exp(i\alpha r_{12}) \alpha_1 \alpha_2 / r_{12}$ of the inter particle interaction. The cross-section is $\sigma = -2 \text{Im}\Delta E$. We have carried out a detailed studying the collision cross-sections and collision strengths (the incident electron energies 0.425, 0.5, 0.75, 1.045 keV) for Ne-like ions CIVIII, ArIX, CaXI, TiXIII, CrXV from the ion ground state to a set of excited states ($2s_{1/2}2p_{1/2,3/2}$, $2p_{3/2,1/2}3s_{1/2}$, $2p_{3/2,1/2}3p_{3/2,1/2}$, $2p_{3/2,1/2}3d_{5/2,3/2}$, $2s_{1/2}3s_{1/2}$, $2s_{1/2}3p_{1/2,3/2}$, $2s_{1/2}3d_{3/2,5/2}$ [$J=0,1,2,3,4$]) and Ar-like ion of Ba (the incident electron energy 5.8, 9.5 keV), for majority of which there are absent exact data. To test the results of calculations we compare the obtained data for Ne-like ions of Fe, Ar with other authors' calculations and available experimental data. The inclusion of Na-like states, accounting for diffusion-like processes, can increase the population inversion for the "lasing candidates" by at least a factor of two for a wide range of plasma conditions.

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