R-MATRIX CALCULATION OF THE ELECTRON-IMPACT EXCITATION OF Zn^+ AND Cd^+

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This work presents the calculations of the excitations cross-sections for electron scattering on Zn^+ and Cd^+. The low-energy electron impact excitation of Zn^+ and Cd^+ are investigated using the R-matrix method. Excitation cross section calculated in R-matrix approximation are compared with the existing atomic-collision experiments. The most particular attention we have paid to the accuracy of the target-state wavefunctions where both the core-valence correlation and the relaxations are shown to be important. The calculated date reveal a large resonance contribution in the low-energy region, which is more prominent in comparison with other one-electron-like ions.

Our R-matrix calculations of the electron-impact excitations of Zn^+ and Cd^+ ions were initiated by the recent measurements in Institute of Electron Physics [1,2]. In these works the 4p-4s emission cross sections for Zn^+ differ noticeably in the near-threshold region from the previous cross-beam measurements [3], and considerably differ for all energies from measurements [4].The accuracy of the existing *R*-matrix calculations [5] does not allow one to give a complete interpretation for the above measurements. This group [1, 2] also carried out additional $e^- + Cd^+$ measurements. As a results, they succeeded in detecting the strong resonance structure in the near-threshold region. The energy behaviour of the obtained emission cross sections for the resonance 5s-5p transition differ considerably from the results [6], who carried out the first measurements of the electron-impact excitation cross sections in Cd^+. The peak value of the cross section for the resonance 5p - 5s line is 3 times larger than the maximum cross section for the similar 4p-4s transition in Zn^+. Up to the last time there have been no reports on the quantum mechanical calculations of electron excitation in Cd^+ which can be used to interpret the above measurements. We have first presented the R-matrix calculations of the $e^- + Cd^+$ process.

Now there are many methods which are able to describe perfectly the electron scattering by the one-electron-like atoms where the target wave functions can be obtained with a high accuracy analytically or by using some model potentials. For the complex atoms, especially for those with some open shells, the accurate representation of the target wave functions becomes equally important. The existing published scattering codes are not very well adapted for such cases, and the usual practice is to use the possibly simplest target wave functions, because the use of the extensive multiconfiguration expansions considerably complicates the scattering calculations. The presence of the subvalent 3d-shell in Zn^+ and 4d-shell in Cd^+, which have the average radiuses and excitation energies close to those for the outer valence electrons, leads to a strong core-valence correlation. Indication of this is the large difference between the Hartree-Fock and experimental binding energies for low-lying states for these elements. For Cd^+ ion discrepancies from Hartri-Fock calculation and experimental values are even more large as compared to the case of Zn^+ ion. This indicates that the core-valence correlation and relaxation effects increase with nuclear charge. As expected, the relativistic effects also become more important for Cd^+. The inclusion of core-valence correlation can strongly influence the low-energy cross sections, especially, that concerns the resonance structure. For this reason, the main attention

we have been paid to the accurate representation of the target states To do this, we used the extensive MCHF wave functions to describe the targets. Of particular difficulty here is the determination of the energy positions of the Rydberg $3d^{10}nl$ and core-excited $3d^9n'l'n''l''$ states for Zn^+ and $4d^{10}nl$ and core-excited $4d^9n'l'n''l''$ states for Cd^+ in the same basis. The corresponding corrections are very large, especially for the core-excited states, and strongly influence the relative positions of the target states. We have found that the relaxation is connected both with the large changes in the outer orbitals and with the relatively large change of the subvalent orbital itself. Therefore, the accurate representation of the target wavefunctions requires the simultaneous inclusion of both the core-valence correlation and the relaxation effects, and all the target and scattering calculations for Zn^+ and Cd^+ have been performed in the *LS*-coupling with the inclusion of the relativistic shift terms in the atomic Hamiltonian.

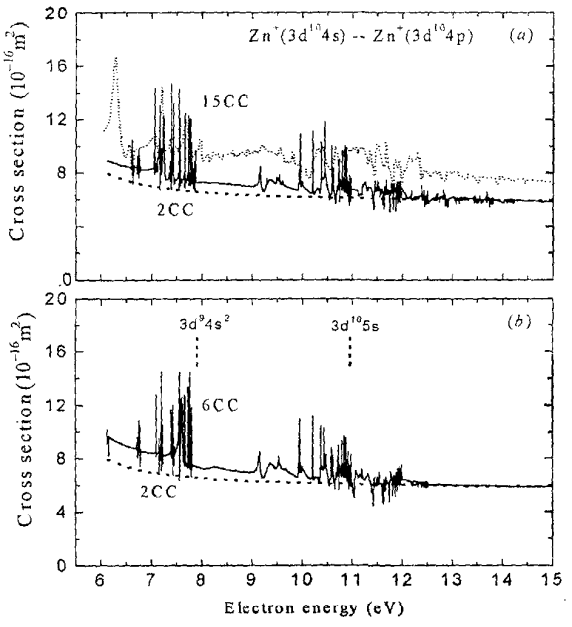

Fig. 1. The 4s-4p excitation cross section in Zn^+. Solid curves represent the R-matrix results obtained in the 15-state approximation (15CC), layer (*a*), and in the 6-state approximation (6CC), layer (*b*). Dashed curves represent the two-state results (2CC), scaled by a factor of 0.833. Comparison is given with the 15-state close-coupling calculations [5], dotted symbols, layer (*a*).

The collision cross sections were calculated in the 15-states close-coupling approximation (15CC) using the *R*-matrix method. For completeness, we also carried out the 6CC and 2CC calculations, in order to evaluate the influence of coupling between the scattering channels on the excitation cross sections and to examine the convergence of the close-coupling expansion. To indicate the resonance contribution and the close-coupling effects, Figs. 1, 2 also contain the 2CC cross sections normalized to the 15CC results. This value characterizes the overall influence of channel coupling in the low-energy region. The 6CC results repeat essentially the general structure of the 15CC cross sections, with the absence of some resonances and with some small shifts of low-lying resonances toward the higher energies.

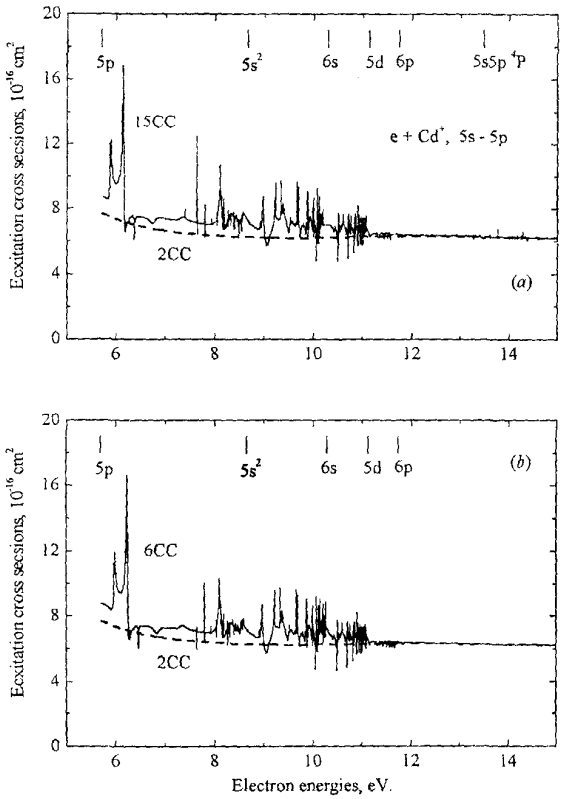

Fig. 2. The 5s-5p excitation cross section in Cd^+. Solid curves represent the R-matrix results, obtained in the 15-state approximation (15CC), layer (*a*), and in 6-state approximation (6CC), layer (*b*). Dashed curves represent the two-state results (2CC), scaled by factor 0.836.

The calculated cross sections for the 5s-5p transition for Cd^+ show a rich resonance structure, is more intensive in comparison with the 4s-4p transition in Zn^+. A distinct feature of the resonance structure for Cd^+ is that two resonances, $4d^95s^25p\ ^3P^o$ and $^3F^o$, are clearly stand out in the near-threshold region. As is seen from Figure 2, the main resonance contribution to the 5s-5p transition arises from the $4d^{10}6snl$ autoionizing states, a considerably smaller contribution arises from the $4d^{10}5dnl$ states, and a negligibly small contribution is due to the higher-lying autoionizing states. Such behaviour is expected because the higher-lying autoionizing states decay dominantly to the nearest Cd^+ levels, and there is only a small probability for the population of the low-lying states.

Fig. 3,4 compares the 15CC cross sections with the experimental data. In [1,2] authors measured the cross sections for the individual components of the $^2P_{1/2,3/2}$ doublets. The near-threshold resonance structures for these components differ markedly from each other, and the cross sections presented in Fig. 3,4 were obtained by a graphical summation of the data for the individual components. These data are relative, and were normalize on the 15-state calculations at 30 eV for Zn^+ and at 40 eV Cd^+. As is seen from Figures 3,4, these measurements show a considerably more strong resonance structure than it can be expected from the calculations. Hence, a direct comparison of the *LS* results on the resonance positions with the experimental data has no sense, but the obtained resonance structure can only be considered as the indication of the total resonance contribution to the excitation cross sections. The discrepancy in the near-threshold region for Cd^+ has the same character as in the case of $e^- + Zn^+$ scattering. More severe and detailed comparison could be done for the cross sections of individual components, but this requires the inclusion of the spin-orbit mixing in the close-coupling calculations. For Zn^+ we obtained excellent agreement with the crossed-beam absolute measurements [3]. For Cd^+ the absolute measurements [6] can not serve as a test in our case, because they have large uncertainty (45%) and were carried out with an uncontrolled electron-energy spread. Besides, they gives too large cross sections, which exceed the present data more than 3 times. It is worth also to note the large cascade contribution to the 4s-4p for Zn^+ and 5s-5p for Cd^+ cross sections. The overall cascade contribution can be estimated within the limits of 20% .

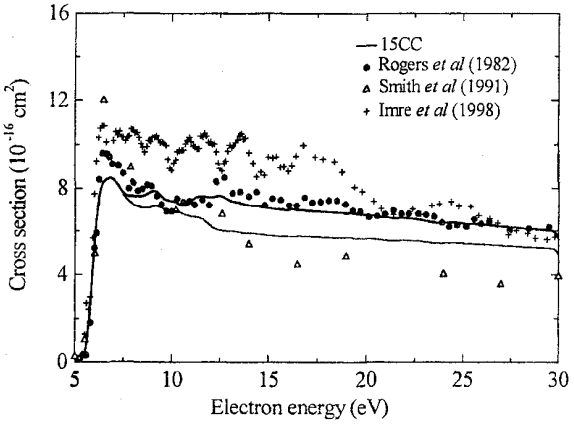

Fig. 3. A comparison of the 4s-4p excitation cross sections in Zn^+ with the experimental data. The lower solid curve represents the 15CC R-matrix calculations, the upper one includes the cascade contribution.

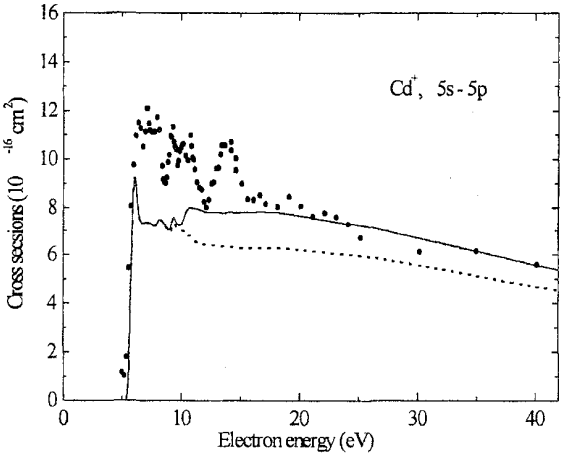

Fig. 4. A comparison of the 5s-5p excitation cross sections in Cd^+ with the experimental data [2](solid circles). The dotted curve represents the 15CC *R*-matrix calculations, the solid curve include also the cascade contribution. The theoretical cross sections are convoluted with the energy spread equal 0.2 eV FWHM.

As a conclusion, the calculations and the experimental data reveal a large resonance contribution in the low-energy region of e^- +

Cd^+ scattering, which is more prominent in comparison with $e^- + Zn^+$ scattering and the other one-electron-like ions. This can be attributed to the influence of the subvalent shells, which have relatively small excitation energies and whose excitation leads to a strong resonance structure. However, up to now there are the large discrepancies concerning both the absolute values and the resonance contribution between the existing measurements and the *R*-matrix calculations. In general, the further development of the atomic-collision experiments, especially with respect to the mapping out of the resonance structure at high resolution, can provide a strong test of the present techniques for the computation of the atomic structure and collisional dynamics. Our *R*-matrix calculations show also that the adequate description of the $e^- + Zn^+$ and $e^- + Cd^+$ scattering requires the simultaneous inclusion of the electron correlation and relativistic corrections that is yet an unsolved task in the modern computational physics in the case of an arbitrary complex atom.

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R-МАТРИЧНІ РОЗРАХУНКИ ЗБУДЖЕННЯ Zn^+ ТА Cd^+ ЕЛЕКТРОННИМ УДАРОМ

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В роботі представлено R-матричні розрахунки перерізів збудження іонів Zn^+ та Cd^+ електронним ударом. Отримані значення перерізів порівняно з існуючими експериментальними результатами. Найбільшу увагу приділено точності розрахунків хвильових функцій мішені, показано важливість врахування як ефектів релаксації, так і кореляції. Для області низьких енергій розрахунки дали більш виражену резонансну структуру в порівнянні з іншими іонами з одним зовнішнім електроном.