

**ELECTRON TRANSFER IN COLLISIONS BETWEEN  
HEAVY ELEMENT IONS, ALPHA-PARTICLES, AND  
HELIUM ATOMS IN PLASMA AND IN BEAMS**

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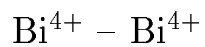
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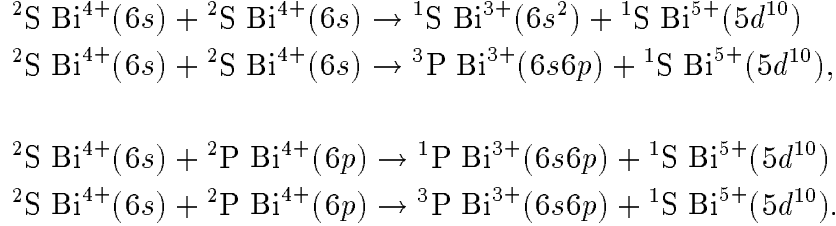
V RESEARCH PROPOSAL:

“ELECTRON TRANSFER AND EXCITATION IN COLLISIONS  
BETWEEN HEAVY ELEMENT IMPURITY IONS AND  
HELIUM ATOMS”

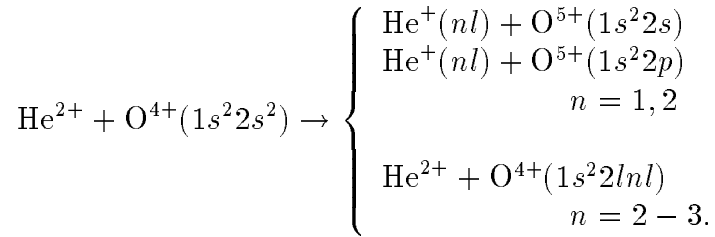
## Summary

Some recent results of theoretical studies of charge transfer in collisions involving heavy element ions and alpha-particles and proposed research project will be reviewed.

Charge-changing collisions between ions within the beams occur at keV relative transverse energies due to betatron oscillations. Coupling-state molecular treatment of charge-transfer in slow collisions between quadruply charged bismuth ions in ground and metastable states was performed.



Cross sections for charge transfer in collisions of alpha-particles with the beryllium-like oxygen ions were calculated by using the close-coupling equation method with the basis set of thirteen four-electron quasi-molecular states in the collision energy range 20 keV – 2 MeV.



The main aim of the proposed research is to provide new theoretical data on the electron transfer and excitation processes in collisions of the multiply charged metallic impurity ions of elements Ti, Cr, Fe, Ni, Mo, and W important to present CRP with helium atoms in the ground as well as in the initially excited states. The single and double electron capture, transfer excitation, and excitation of helium will be calculated at relative keV-collision energies important for modeling and diagnostics of the plasma edge. We plan to study inverse reactions of alpha-particles neutralization in their collisions with metallic ions through the quasi-resonant double electron capture which may be important in cooling of plasmas containing alpha-particles. The calculations will be carried out by using our computer program package for the treatment inelastic processes in slow ion-atom collisions in the framework of the close-coupling equation method involving basis set of many-electron quasi-molecular states.

## II. Theoretical method

The study of charge transfer and excitation reactions was performed by the use of the close-coupling equation method with two- or many-electron quasi-molecular states  $\phi_i$  as a basis. Coulomb trajectories were used to integrate coupled equations using code TANGO provided us by A. Salin.

Two-electron wave function  $\phi_i$  for the orthonormal one electron basis  $\psi_k$  may be represented in form

$$\phi_i(\vec{r}_k, \vec{r}_l) = \frac{1}{\sqrt{2}}[\psi_k(\vec{r}_k)\psi_l(\vec{r}_l) \pm \psi_k(\vec{r}_l)\psi_l(\vec{r}_k)] \quad (\pm - \text{singlet, triplet cases}), \quad (2.1)$$

where  $\psi_k$  may be obtained within effective potential method. The our effective potential takes into account a screening of a nucleus by electrons

$$V_{eff}(R, \vec{r}_j) = \frac{1}{2} \left[ \frac{a_1 - b_1}{r_{1j}} + \frac{a_1 + b_1}{r_{2j}} + \frac{\tilde{a}_1 + Ra_0}{r_{1j}r_{2j}} + \frac{b_2(r_{1j} - r_{2j})^2}{Rr_{1j}r_{2j}} \right] \quad (2.2)$$

and allows for the separation of variables in one-electron Schödinger equation in prolate spheroidal coordinate system

$$h\psi_k(\vec{r}_j) = \left[ -\frac{\nabla_j^2}{2} - \frac{Z_1}{r_{1j}} - \frac{Z_2}{r_{2j}} + V_{eff}(\vec{R}, r_{1j}, r_{2j}) \right] \psi_k(\vec{r}_j) = \varepsilon_k(R)\psi_k(\vec{r}_j), \quad (2.3)$$

where  $R$  is the internuclear distance and  $r_{1j}$  and  $r_{2j}$  are the distances from the  $\vec{r}_j$  electron to the nuclei with charges  $Z_1$  and  $Z_2$ , respectively. The scheme for determining the effective potential parameters  $a_0$ ,  $\tilde{a}_1$ ,  $a_1$ ,  $b_1$  and  $b_2$  are given in our papers.

If  $V_{eff}=0$  we have  $H_2^+$  problem and One Electron Diatomic Molecular Orbitals (OEDMO) with hidden symmetry. In our method Screened Diatomic Molecular Orbitals (SDMO),  $\psi_k$  have the same symmetry.

The SDMO basis was used for calculating the total energies  $E_i$  for example of the two-electron or many-electron diabatic states

$$E_i = \langle \phi_i | H | \phi_i \rangle = \varepsilon_k + \varepsilon_l + J_{kl}^c \pm J_{kl}^{ex} - (V_{eff}^k + V_{eff}^l), \quad (2.4)$$

$$H = \sum_{j=k,l} \left[ -\frac{\nabla_j^2}{2} - \frac{Z_1}{r_{1j}} - \frac{Z_2}{r_{2j}} \right] + \frac{1}{r_{kl}}. \quad (2.5)$$

Here  $J_{kl}^c$ ,  $J_{kl}^{ex}$  are Coulomb and exchanged integrals;  $V_{eff}^k$  and  $V_{eff}^l$  are diagonal matrix elements of the effective potential.

The many-electron energies are calculated in fact to the first order of perturbation theory in residual interaction  $W=1/r_{kl} - V_{eff}(\vec{r}_k) - V_{eff}(\vec{r}_l)$ .

The matrix elements of dynamic and potential couplings are obtained using the calculated basis SDMO. The dependence of results on origin of electronic coordinates at dynamic matrix element calculations has been investigated. All final results for matrix elements have been obtained for origin placed at centre of charges of colliding ions.

### III. Coupled-state molecular treatment of charge-transfer in slow heavy ion-ion collisions: $\text{Bi}^{4+} - \text{Bi}^{4+}$

#### 1. Introduction

The study of charge transfer in collisions between identical heavy ions is relevant to efficiency of future accelerators and storage rings. Charge-changing collisions between the ions within the beams occur at keV relative transverse energies due to betatron oscillations. Recently the total charge transfer cross sections for collisions between quadruply charged bismuth ions were measured by Erhard Salzborn et al. and expected particle losses due to such collisions from 100 Tm synchrotron were estimated [3.1,3.2].

An uncertainty in experimental data [3.1,3.2] may be due to the presence in the crossed beams of ions in metastable states which yield a larger cross sections compared with the ions in the ground state. In this case the experimental values of transfer cross sections should be larger than the theoretical data. The reasonable estimate of the fraction of metastable ions can be obtained from the comparison of experimental and the theoretical data. The only available results of calculation by Shevelko [3.3] for  $\text{Bi}^{4+} - \text{Bi}^{4+}$  collisions are even in qualitative disagreement with experimental data [3.1,3.2]. The calculations [3.3] are based on OBK approximation, the fundamentally two-active electron collisional system  $\text{Bi}^{4+}(6s) - \text{Bi}^{4+}(6s)$  being considered as system with one active electron and the hydrogen-like wave functions with bare effective charges are used for the target and the projectile.

#### 2. Results

The purpose of our study was two-electron multi-state calculation of charge transfer and excitation cross section for collisions:

- (1)  ${}^2\text{S Bi}^{4+}(6s) + {}^2\text{S Bi}^{4+}(6s) \rightarrow {}^1\text{S Bi}^{3+}(6s^2) + {}^1\text{S Bi}^{5+}(5d^{10}), \Delta E_1 = 11,64 \text{ eV}$
- (2)  ${}^2\text{S Bi}^{4+}(6s) + {}^2\text{S Bi}^{4+}(6s) \rightarrow {}^3\text{P Bi}^{3+}(6s6p) + {}^1\text{S Bi}^{5+}(5d^{10}), \Delta E_2 = 20,27 \text{ eV}$
  
- (3)  ${}^2\text{S Bi}^{4+}(6s) + {}^2\text{P Bi}^{4+}(6p) \rightarrow {}^1\text{P Bi}^{3+}(6s6p) + {}^1\text{S Bi}^{5+}(5d^{10}), \Delta E_3 = 10,44 \text{ eV}$
- (4)  ${}^2\text{S Bi}^{4+}(6s) + {}^2\text{P Bi}^{4+}(6p) \rightarrow {}^3\text{P Bi}^{3+}(6s6p) + {}^1\text{S Bi}^{5+}(5d^{10}), \Delta E_4 = 10,44 \text{ eV}$

Here  $\Delta E_{1,2}$  are the energies of resonance defect of charge transfer obtained from ionic total energy Hartree-Fock-Dirac (HFD) calculations. For triplet collisions the energy of resonance defect is more higher ( $\Delta E=20, 27 \text{ eV}$ ) and therefore they were discarded in our preliminary study [3.4] (as well as reactions (3) and (4)). The study of charge transfer and excitation for reactions was performed within the framework of the method of perturbed

stationary states. We adopted the five-state CI gerade and ungerade screened diatomic molecular orbital (SDMO) expansion to obtain the transition amplitude in the impact parameter approach.

The energies of four orthonormal SDMO ( $6s\sigma$ ,  $7p\sigma$ ,  $7d\sigma$ ,  $8f\sigma$ ) were obtained within the effective potential method. Our effective potential takes into account a screening by electrons of the separated and united ionic cores. Energies of SDMO were matched to appropriate atomic energies at  $R=0$  and  $R=\infty$  obtained from HFD electronic structure calculations of ions with  $Z=166$  and  $Z=83$  ( $R$  is the internuclear distance).

In Fig. 1 diabatic correlation diagram of  $\text{Bi}^{4+}(6s) + \text{Bi}^{4+}(6p)$  quasi-molecule is given.

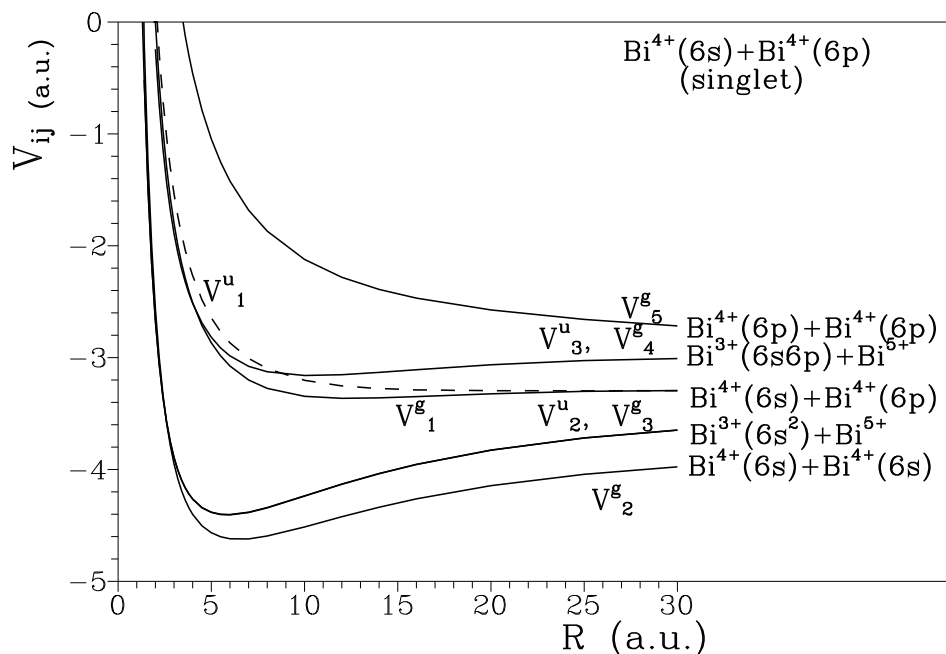


Figure 1: Diabatic correlation diagram of  $\text{Bi}^{4+}(6s) + \text{Bi}^{4+}(6p)$  quasi-molecule.

The results [3.4] of our five-state calculation in the centre-of-mass energy range from 2 to 70 keV of transfer cross section for reactions (1–4) together with experimental data are shown in Fig. 2. It is clearly seen that our results are in a good agreement with the experimental data [3.1,3.2]. It is notable that humped (oscillatory) structure of the cross sections is similar in the shape.

In Fig. 3 the statistically weighted singlet total charge transfer cross sections separately for projectile and target are given for  $\text{Bi}^{4+}(6s) + \text{Bi}^{4+}(6p)$  collision.

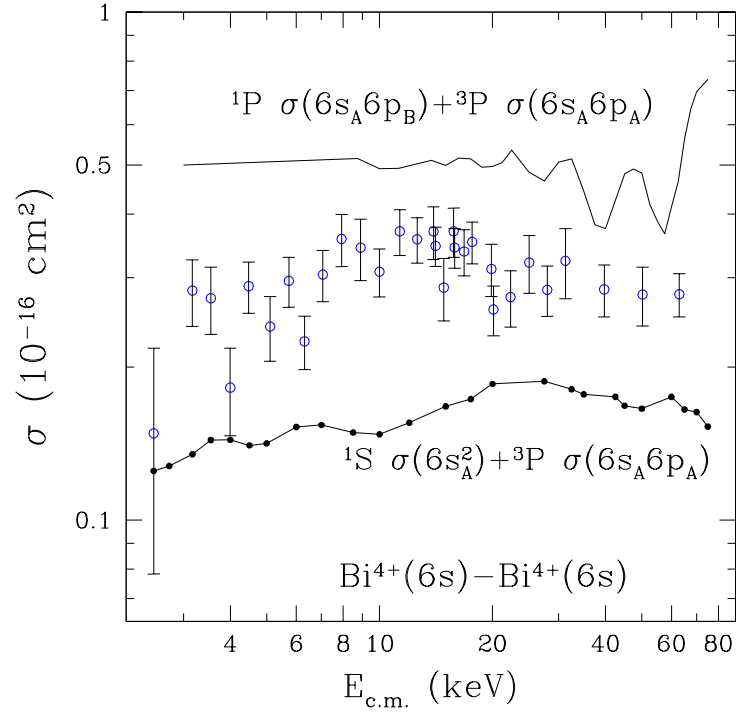


Figure 2: Comparison of our statistically weighted singlet total charge transfer cross sections for reactions(1-2) and for reactions (3-4) with the experimental data (o) for  $\text{Bi}^{4+} + \text{Bi}^{4+}$  collision [3.1,3.2] depending on the centre-of-mass energy.

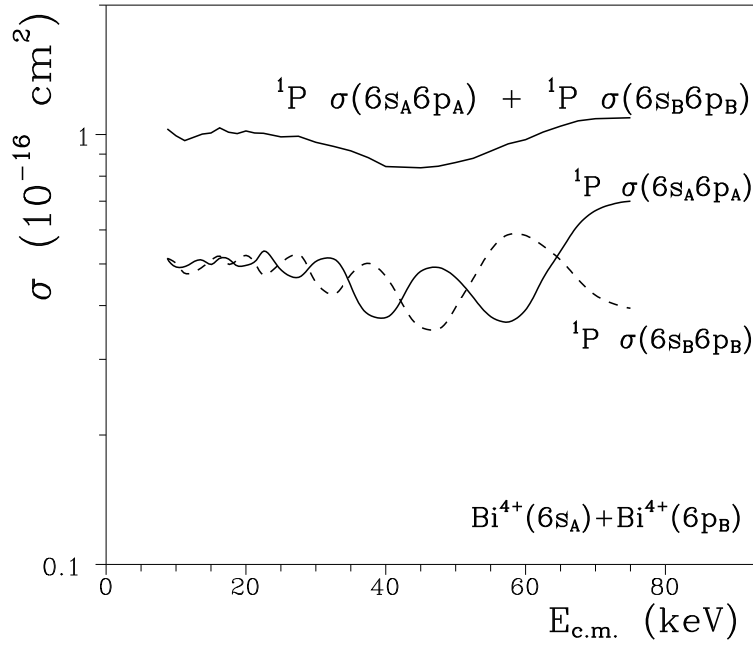


Figure 3: The charge transfer cross-sections for singlet collision  $\text{Bi}^{4+}(6s) + \text{Bi}^{4+}(6p)$ .

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## IV. Electron capture and excitation processes in collisions of alpha-particles with Be-like $O^{4+}$ ions (four-electron quasi-molecule)

The purpose of theory was to obtain reliable data for the first time on total and state-selective cross sections of charge transfer and of excitation processes in collision of alpha-particles with  $O^{4+}$  ions at collision energy from 20 keV to 2 MeV.

The calculations were carried out using the method of close-coupling equations with the basis set of thirteen quasi-molecular four-electron states listed in Table I.

Table I. Entrance ( $j=1$ ), charge transfer ( $j=4,10,11$ ), TE ( $j=5,14,15$ ) and target excitation ( $j=2,3,6-9$ ) channels ( $\Delta E_j$  are energies of resonance defects).

$\Phi_p$	the atomic limit at $R \rightarrow \infty$	$\Delta E_j$ (a.u.)
$\Phi_{12}, \Phi_{13}$	$He^+(2l) + O^{5+}(1s^2 2p)$	$\Delta E_{14,15}=3.97$
$\Phi_9$	$He^{2+} + O^{4+}(1s^2 2p 4f)$	$\Delta E_9=3.84$
$\Phi_{10}, \Phi_{11}$	$He^+(2l) + O^{5+}(1s^2 2s)$	$\Delta E_{10,11}=3.59$
$\Phi_8$	$He^{2+} + O^{4+}(1s^2 2s 4f)$	$\Delta E_8=3.41$
$\Phi_7$	$He^{2+} + O^{4+}(1s^2 2p 3d)$	$\Delta E_7=3.19$
$\Phi_6$	$He^{2+} + O^{4+}(1s^2 2s 3d)$	$\Delta E_6=2.75$
$\Phi_5$	$He^+(1s) + O^{5+}(1s^2 2p)$	$\Delta E_5=2.17$
$\Phi_4$	$He^+(1s) + O^{5+}(1s^2 2s)$	$\Delta E_4=2.05$
$\Phi_3$	$He^{2+} + O^{4+}(1s^2 2p^2)$	$\Delta E_3=0.96$
$\Phi_2$	$He^{2+} + O^{4+}(1s^2 2s 2p)$	$\Delta E_2=0.48$
$\Phi_1$	$He^{2+} + O^{4+}(1s^2 2s^2)$	$\Delta E_1=0$

Energies of many-electron quasi-molecular states and matrix elements (dynamic and potential) were calculated using our program package for a treatment of inelastic processes at ion-atom collision in a framework of the quasi-molecular approach.

The results of our calculation [4.1] of charge transfer and transfer excitation for  $He^{2+} - O^{4+}(1s^2 2s^2)$  collision are shown in Fig. 4. Simultaneous transfer and excitation (TE) of two electrons in  $He^{2+} - O^{4+}(1s^2 2s^2)$  collision is an

example of correlation process. It is apparent from Fig. 4 that TE process is of importance for charge transfer process. It is notable that oscillatory structure of charge transfer cross sections in  $\text{He}^{2+} - \text{O}^{4+}(1s^2 2s^2)$  and in  $\text{He}^{2+} - \text{C}^{4+}(1s^2)$  collisions are similar in the shape.

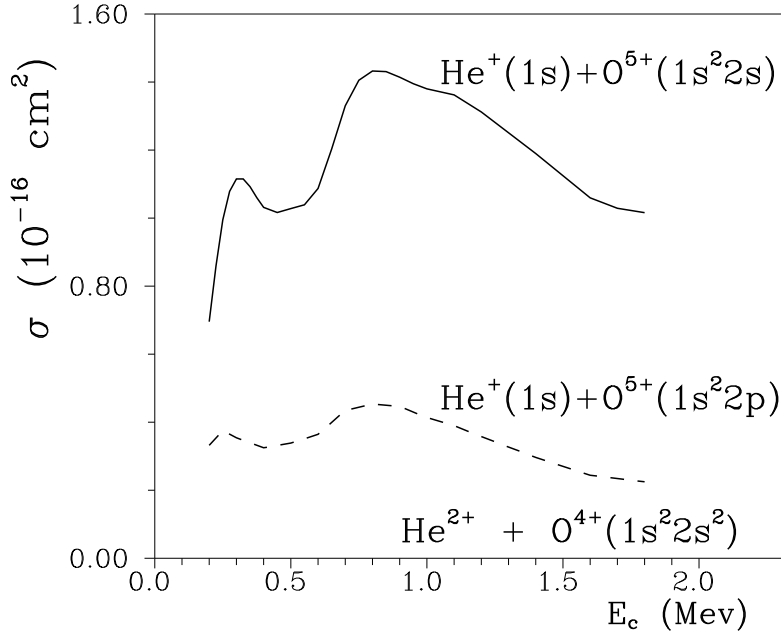


Figure 4: The charge transfer and TE cross-sections for collision of alpha-particles with Be-like ions  $\text{O}^{4+}$ .

For comparison with the results in Fig. 4, the results of our previous [4.2] two-electron multistate calculation of charge transfer cross section for  $\text{He}^{2+} - \text{C}^{4+}(1s^2)$  collision together with indirect experimental data (by M. Rodbro, E.H. Pedersen, C.L. Cocke et. al, Phys. Rev. A 19, 1936 (1979)) on  $1s - 1s$  capture in the  $\text{He}^{2+} - \text{CH}_4$  collision are shown in Fig. 5. It is clearly seen that our results are in generally good agreement with experimental data. It is notable that the two-humped structures of the cross section curves are similar in shape. Results of our calculation of the cross section without taking into account rotational coupling between  $2p\sigma - 2p\pi$  SDMO are presented in Fig. 5. In this case the structure is disappeared. One might think that the two-humped structure of the cross section curves is associated with this coupling.

In Fig. 5 we compare our results for  $\text{He}^{2+} + \text{C}^{4+}$  collision system with the results of previous calculations communicated in paper by M. Rodbro et al. The results of C.D. Lin (L) are from the close-coupling calculation using basis set of atomic orbitals, while those of Dž. Belkić, R. Gayet and A. Salin (BGS) are from the continuum-distorted-wave calculation. In high velocity limit there is agreement between all theoretical results and experiment.

Charge transfer and TE excitation cross sections onto  $1s, 2s, 2p$  states of  $\text{He}^+$  ion are shown in Fig. 6.

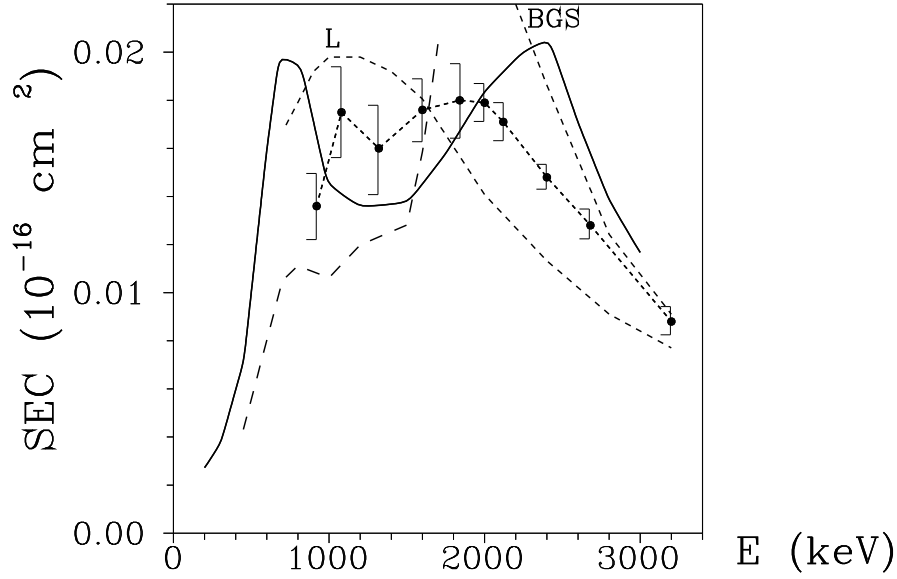


Figure 5: The cross sections for the single-electron capture in  $\text{He}^{2+} + \text{C}^{4+}(1s^2) \rightarrow \text{He}^+(1s) + \text{C}^{5+}(1s)$  collisions. Solid line – our results, broken line – our results without taking into account the  $\langle 2p\sigma | iL_y | 2p\pi \rangle$  rotational coupling;  $\bullet$  – experimental data by M. Rodbro et al; dashed lines – theoretical data by Belkić, Gayet and Salin (BGS) and by Lin (L).

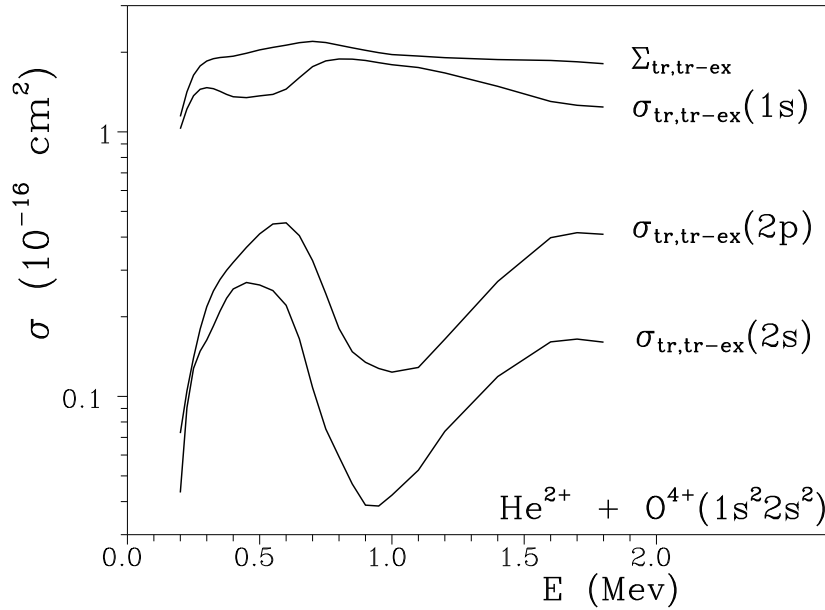


Figure 6: The total and partial charge exchange (transfer plus transfer excitation) cross sections in collision of alpha-particles with Be-like ions  $\text{O}^{4+}$ .

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## V. Research proposal: “Electron transfer and excitation in collisions between heavy element impurity ions and helium atoms”

### 1. Scientific background:

#### a. Significance of overall problem:

Energy loss due to photon emission from metallic impurity ions excited through charge-exchange collisions with hydrogen or helium atoms is a serious problem in fusion reactions. Destruction of ground and especially excited states of abundant neutral atomic and molecular hydrogen and He atoms by Single Electron Capture (SEC) and Double Electron Capture (DEC) in their collisions with metallic impurity ions are the most important processes in the edge plasma.

In inverse reactions slow alpha-particles may be taken away at their neutralization through the quasi-resonant DEC collisions with impurities. This process could be important in cooling of the plasmas containing alpha-particles, since the DEC cross sections may have even larger values than the corresponding SEC ones for some collision systems. This was shown for the first time in our study [5.1] of the alpha-particle neutralization reactions in collision with  $C^{2+}$  ions. DEC transfer into  $He(1s^2)$  ground state in this collision is the dominant process at center mass energies  $< 25$  keV, the SEC channel become dominant at center mass energies above 40 keV.

Previously the key role of the alpha-particle neutralization reactions in cooling the edge plasmas was discussed by Tawara [5.2]. The reactions are due to DEC into metastable  $He^o(1s3l)$  state at collisions of alpha-particles with  $H_2$  at low eV-energies. On the other hand DEC cross sections into  $He^o(1s^2)$  ground state are known to be small [5.2] contrary to our case.

The electron transfer and excitation in collisions between impurities and helium atoms in ground and excited states of atomic beams used for edge and central plasma diagnostics could be important in the level population.

#### b. Related work already performed or in progress at other institutes:

Recently within IAEA projects a serious effort was made by theorists and experimentalists to determine the relevant cross sections involving heavy metallic impurities.

Total transfer cross sections were determined by Katsonis et al [5.3] within the classical-trajectory Monte Carlo method for collisions of  $T^{q+}$ ,  $Cr^{q+}$ ,  $Fe^{q+}$  and  $Ni^{q+}$  ( $4 \leq q \leq Z$ ,  $Z$  being the nuclear charge) with atomic hydrogen in the energy range from 10 to  $10^3$  keV/amu.

Total and partial electron transfer cross sections were determined by Fritsch [5.4] for collisions between atomic hydrogen and the most stable

closed 3p-shell ions of Ti, Cr, and Fe, since ions with unfilled shells are more difficult for study by theory and experiment and are less suitable for plasma diagnosis. The calculations were performed within the framework of the close-coupling method in the energy range from 0.5 to 100 keV/amu.

The experimental and theoretical data in collision of heavy metallic ions with neutral helium atoms is very limited or even, as data on elements Mo, W is lacking [5.5, 5.6]. To our knowledge there are only two theoretical works involving multiply charged metallic ions. McLaughlin et al [5.7] have carried out multi-channel Landau- Zener calculations for  $\text{Fe}^{4+}$ - He collisions in low keV energy range which provide only a qualitative description of experimental data. The calculations of total and partial cross sections for  $\text{Ti}^{4+}$ - He collisions in the energy range 0.1–6 MeV were performed by Fritsch [5.8] within the framework of the close-coupling method and taking into consideration two active electrons, the important two-electron transfer excitation and DEC channels being omitted from calculations.

2. Scientific scope of the project and work plan for first two years including proposed methods:

The purpose of the project is to obtain the theoretical data on the electron transfer and excitation processes in slow collisions of multiply charged metallic impurity ions with the neutral helium atoms which is required for diagnostics and the modeling of fusion plasmas. The specific objectives of the project are the following:

- (i) To calculate for above-mentioned collisions cross sections for SEC and for electron transfer with excitation of helium ion (transfer excitation) as well as for DEC and true excitation of helium. The calculations will be performed for metallic and some other impurity ions of elements important for the present CRP (C, O, Ti, Cr, Fe, Ni, Mo, W, Bi).
- (ii) To obtain the DEC, SEC and true excitation cross sections in slow collisions of impurity ions with helium  $\text{He}(1s2s) 2^1\text{S}$  in initially excited state. The excitation cross sections may have even larger values than the corresponding electron-impact cross sections.
- (iii) To reveal inverse reactions with neutralization of alpha-particles through the quasi-resonant DEC collisions with specific metallic impurity ions.

In the first two years we intend to reassess critically the available data information for charge transfer and excitation processes with the aim to identify the specific metallic impurity ions for which data are of a prime necessity in the study of plasma modeling and in the diagnostics.

- (i) The detailed theoretical study will be made of state-selective single- and double-electron capture, transfer excitation and true helium excitation in collisions of closed shell  $\text{Ti}^{4+}$ ,  $\text{Cr}^{6+}$ , and  $\text{Fe}^{8+}$  ions with helium in the ground as well as in the excited  $\text{He}(1s2s) 2^1\text{S}$  states.

The relative collision energies will be in keV range, i.e. energies prevailing

in the plasma edge and typical for the low-energy of neutral He beams used for the edge plasma diagnostics.

Special attention will be paid to the study of true DEC and of the inverse reactions of alpha-particles neutralization through the quasi-resonant DEC in their collisions with metallic impurities.

For example, two-electron state correlation diagram for  $\text{Ti}^{4+} + \text{He}(1s^2)$  quasi-molecule is shown in Fig. 7. It is clearly seen that DEC may proceed through intermediate SEC channel.

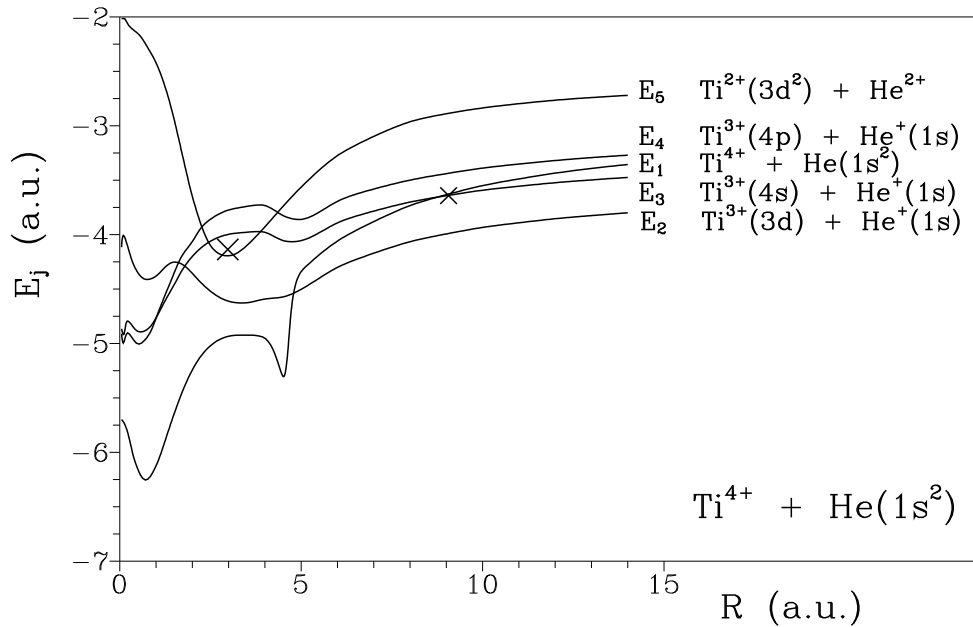


Figure 7: The energies  $E_j$  of two-electron states  $\phi_j$  for  $(\text{Ti}^{4+}+\text{He})$  quasi-molecule: a. Entrance channel –  $\phi_1(3d\sigma, 3d\sigma)$ ; b. SEC channels –  $\psi_2(3d\sigma, 4f\sigma)$ ,  $\psi_3(3d\sigma, 4s\sigma)$ ,  $\psi_4(3d\sigma, 4p\sigma)$ ; c. DEC channel –  $\psi_5(4f\sigma, 4f\sigma)$ .

(ii) The further study of alpha-particle slow collisions with  $\text{C}^{2+}$  ions and with  $\text{O}^{4+}$  ions in MeV energy range will be made.

(iii) Theoretical cross sections of charge transfer and excitation in collisions between quadruply charged bismuth ions within the beams will be obtained.

The detailed study will be made of these collisions by using close-coupling equation method with two-electron quasi-molecular states as a basis. Two-electron states will be obtained in the single configuration approximation with the basis set of Screened Diatomic Molecular Orbitals

(SDMO) calculated by our effective potential method. The matrix elements of dynamic and potential couplings will be obtained using the calculated basis of SDMO. The calculation will be carried out by using our program package for the inelastic process computation in slow ion-atom collisions [5.9]

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