Theoretical study of electron capture and excitation processes in collisions of alpha-particles with helium-like C^{4+}, N^{5+}, O^{6+} ions

V.K. Nikulin, N.A. Guschina
A.F. Ioffe Physical-Technical Institute,
St. Petersburg, Russian Federation

Abstract. The cross section database for the processes of single-electron capture and neutralization of alpha-particles in collisions with helium-like C^{4+}, N^{5+}, O^{6+} ions was produced. The evaluated data were tabulated also for the excitation cross sections of the enumerated He-like ions which are of special importance for fusion research. The maximum values of single-electron capture cross sections were obtained equal to $\sim 2{\cdot}10^{-18}$, $6{\cdot}10^{-19}$, $3{\cdot}10^{-20}$ cm^2 for C^{4+}, N^{5+} and O^{6+} ions, respectively. The maximun values of neutralization cross sections were obtained equal to $4{\cdot}10^{-20}$, $2{\cdot}10^{-21}$, $7{\cdot}10^{-22}$ cm^2 and excitation cross sections were obtained equal to $4{\cdot}10^{-16}$, $2{\cdot}10^{-16}$, $1{,}5{\cdot}10^{-16}$ cm^2.

1. Introduction

The ion-ion collision systems are less suitable for experimental study and there is increasing demand of appropriate data for nuclear-fusion research and astrophysics.

The purpose of our study was to produce cross section databases for the processes of Single-Electron Capture (SEC), Double-Electron Capture (DEC) and of state selective target excitation cross section for collisions of alpha-particles with C^{q+}, N^{q+}, O^{q+} ions – the main impurities released from tokamak surfaces in the form of CO and nitrogen molecules. The study was made of the following reactions in the energy range 20 keV – 3, 4, 5 MeV (depending on whether the velocity of the projectile is lower than that of target electrons):

$$He^{2+} + A^{(Z-2)+}(1s^2) \quad \rightarrow \quad He^{+}(1s) + A^{(Z-1)+}(nl) \ , \tag{1}$$

$$He^{2+} + A^{(Z-2)+}(1s^2) \quad \rightarrow \quad He(1s^2) + A^{Z+} \ , \tag{2}$$

$$He^{2+} + A^{(Z-2)+}(1s^2) \quad \rightarrow \quad He^{2+} + A^{(Z-2)+}(nl, n'l') \ , \tag{3}$$

where $A^{(Z-2)+}$, $A^{(Z-1)+}$, A^{Z+}, respectively, indicate the helium-like, hydrogenic-like and fully stripped ions for atoms C, N and O. If in reaction (1) nl $\neq$ 1s, we have the transfer excitation (TE) process.

The case of alpha-particle projectiles is important for understanding α-losses to walls in TFTR. Particularly important could be the DEC processes which may lead to alpha-particle escape from the central plasma before their complete thermolization. The intensities of emission lines arising from transitions in He-like excited ions are used to determine the electron temperature of fusion plasma.

2. Proposed method

The detailed study of the above reactions was performed by using the close-coupling equation method with nine two-electron quasimolecular states ϕ_i as a basis.

Two-electron states ϕ_i were calculated in the single configuration approximation

$$\phi_i(\vec{r}_k, \vec{r}_l) = \frac{1}{\sqrt{2}}(\psi_k(\vec{r}_k)\psi_l(\vec{r}_l) + \psi_k(\vec{r}_l)\psi_l(\vec{r}_k)) \tag{4}$$

with the basis set of ψ_j (j=k, l) – Screened Diatomic Molecular Orbitals (SDMO), calculated by solving the two-centre problem

$$H\psi(\vec{r}_j) = \left[-\frac{\nabla^2}{2} - \frac{Z_1}{r_{1j}} - \frac{Z_2}{r_{2j}} + V_{eff}(\vec{R}, r_{1j}, r_{2j})\right]\psi(\vec{r}_j) = \varepsilon_j(R)\psi(\vec{r}_j)\ . \tag{5}$$

Here $\varepsilon(R)_j$ – the energies of SDMO. The effective potential $V_{eff}(\vec{R}, r_{1j}, r_{2j})$ is specified [1] in the parametric form

$$V_{eff}(\vec{R}, \vec{r}_j) = \frac{1}{2}\left[\frac{a_1 - b_1}{r_{1j}} + \frac{a_1 + b_1}{r_{2j}} + \frac{\widetilde{a}_1 + Ra_0}{r_{1j}r_{2j}} + \frac{b_2(r_{1j} - r_{2j})^2}{Rr_{1j}r_{2j}}\right]\ , \tag{6}$$

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 ans Z_2, respectively. The scheme for determining the effective potential parameters a_0, $\widetilde{a}_1$, a_1, b_1 and b_2 are given in [1]. The SDMO basis obtained was used for calculating the total energies E_i of the two-electron diabatic states

$$E_i = <\phi_i|H|\phi_i>\ , \tag{7}$$

$$H = \sum_{j=k,l}\left(-\frac{\nabla_j^2}{2} - \frac{Z_1}{r_{1j}} - \frac{Z_2}{r_{2j}}\right) + \frac{1}{r_{kl}}\ . \tag{8}$$

The two-electron energies are calculated to the first order of perturbation theory [2] in residual interaction $W=1/r_{kl}-V_{eff}(r_k)-V_{eff}(r_l)$. The effect of electron screening is important in two-electron quasimolecules.

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

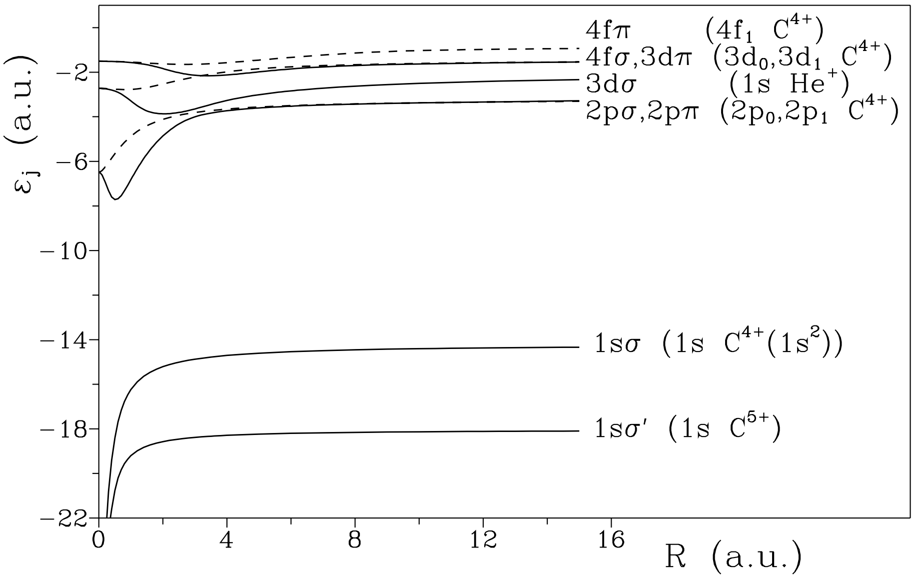

FIG. 1. The energies ε_j of the SDMO for the (He+C)$^{6+}$ quasimolecule.

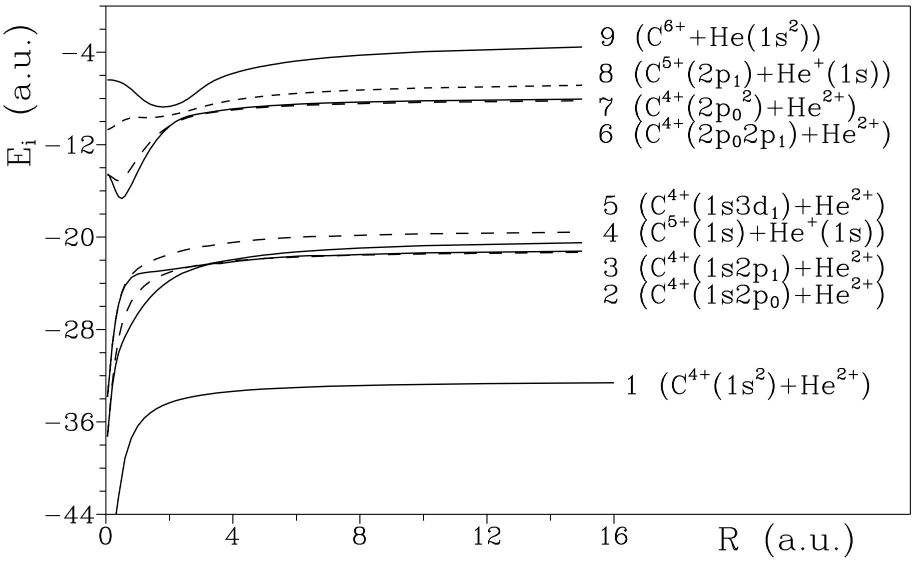

FIG. 2. The energies E_i of two-electron states ϕ_i (i=1 – 9) for the (He+C)$^{6+}$ quasimolecule: a. Entrance channel – $\phi_1(1s\sigma, 1s\sigma)$; b. SEC channel – $\phi_4(1s\sigma', 3d\sigma)$; c. Transfer excitation channel – $\phi_8(3d\sigma, 2p\pi)$; d. DEC channel – $\phi_9(3d\sigma, 3d\sigma)$; e. Single excitation channels – $\phi_2(1s\sigma', 2p\sigma)$, $\phi_3(1s\sigma', 2p\pi)$, $\phi_5(1s\sigma', 3d\pi)$; f. Double excitation channels – $\phi_7(2p\sigma, 2p\sigma)$, $\phi_6(2p\sigma, 2p\pi)$.

The calculated SDMO and two-electron state correlation diagrams for (He+C)$^{6+}$ quasimolecule are shown on figures 1 – 2. The 2pσ–3dσ pseudocrossing (Fig. 1) will be of decisive importance in SEC process in He^{2+}– C^{4+} collision. There is a clear-cut distinction between SDMO and two-electron state correlation diagram as to the concrete 2pσ–3dσ pseudocrossing in Fig. 1 and the corresponding pseudocrossing between ϕ_2 and ϕ_4 states in Fig. 2.

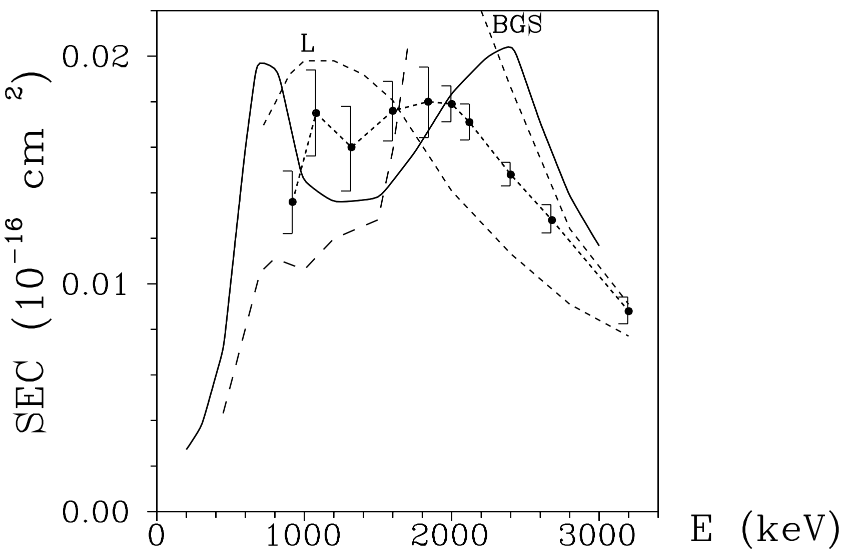

FIG. 3. The cross sections for the single-electron capture in He^{2+} + $C^{4+}(1s^2) \rightarrow He^{+}(1s)$ + $C^{5+}(1s)$ collisions. Solid line – our results, broken line – our results without taking into account $< 2p\sigma|iL_y|2p\pi >$ rotational coupling. • – experimental data by M. Rodbro et al [5]; - - - – theoretical data [5] by Belkić, Gayet and Salin (BGS) and by Lin (L).

3. Results obtained

The results (our preliminary results have been presented early [3], [4]) of our two-electron multistate calculation of SEC cross section for He^{2+}– $C^{4+}(1s^2)$ collision system together with indirect experimental data on 1s – 1s capture in He^{2+} – CH_4 collision [5] are shown in Fig. 3. 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. In Fig. 3 our calculation of SEC cross section is presented without taking into account rotational coupling between 2pσ–2pπ SDMO. In this case the structure has disappeared. One might think that the two-humped structure of the cross section curves is associated with this coupling.

For the same collision systems SEC calculations were reported recently [6] in one-electron two-state approximation. For He^{2+}– O^{6+} system the results by Kuang [6] are an order of magnitude less then ours for alpha-particle energies < 1 MeV .

The results for DEC (reaction (2), neutralization of alpha particles) and for total excitation cross sections (reaction (3)) are shown in Fig. 5 and Fig. 6, respectively.

In Fig. 3 we compare our results for He^{2+}– C^{4+} collision system with the results of previous calculations communicated in work [5]. The results of C.D. Lin (L) are from a close-coupling calculation using basis sets of atomic orbitals (AO), while those of Dź. Belkić, R. Gayet and A. Salin (BGS) are from a continuum-distorted-wave calculation. In the high velocity limit there is agreement between all theoretical results and experiment. For comparison total SEC cross sections for collisions of alpha-particles with He-like C^{4+}, N^{5+}, O^{6+} ions are shown in Fig. 4.

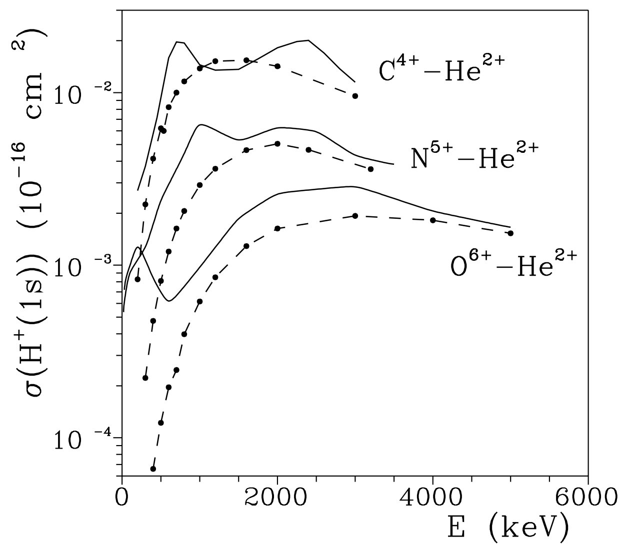

FIG. 4. The comparision of the cross sections for the single-electron capture in He^{2+} + $A^{(Z-2)+}(1s^2)$ collisions for Z=6, 7, 8. Solid line –our results, dash line – data by Y Kuang [6].

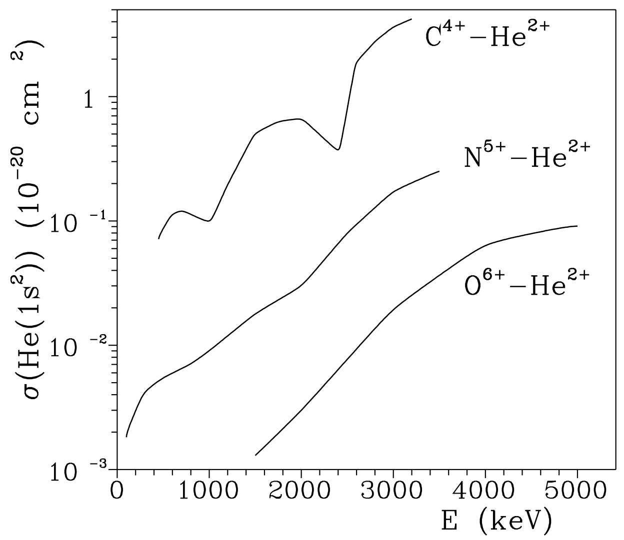

FIG. 5. The cross sections for the double-electron capture in He^{2+} + $A^{(Z-2)+}(1s^2) \rightarrow$ $He(1s^2)$ + A^{Z+} collisions.

The following excitations have been taken into account: C^{4+}(nl,n'l'), N^{5+}(nl,n'l') (where (nl,n'l') $\equiv$ 1s2p$_0$, 1s2p$_1$, 1s3d$_1$, 2p$_0^2$, 2p$_0$2p$_1$; O^{6+}(nl,n'l') (where (nl,n'l') $\equiv$ 1s2p$_0$, 1s2p$_1$, 1s3d$_0$, 2p$_0^2$, 2p$_0$3d$_0$. The dominant contribution to the excitation cross section was found to be the excitations $C^{4+}(1s^2) \rightarrow C^{4+}(1s2p_1)$; $N^{5+}(1s^2) \rightarrow N^{5+}(1s2p_1)$, $N^{5+}(1s2p_0)$; $O^{6+}(1s^2) \rightarrow O^{6+}(1s2p_1)$, $O^{6+}(1s2p_0)$.

The calculated total SEC and transfer excitation cross sections (SEC+TE, reaction 1), DEC cross section (reaction 2) and dominant partial excitation cross sections of He-like target ions $A^{(Z-2)+}(1s^2)$ (reaction 3) are given in Tables 1 – 3.

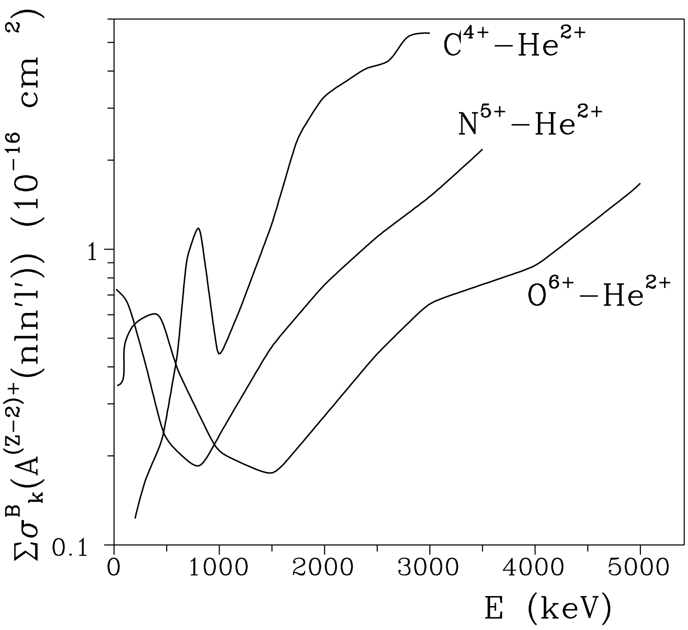

FIG. 6. The total excitation cross sections of He-like target ions $A^{(Z-2)+}(1s^2)$.

Table 1. The total SEC+TE and DEC cross sections and the partial excitation cross sections of $C^{4+}(1s^2)$ ion in He^{2+} – C^{4+} collision

E (keV)	SEC+TE (10^{-16} cm^2)	DEC (10^{-20} cm^2)	$C^{4+}(1s2p_0)$ (10^{-16} cm^2)	$C^{4+}(1s2p_{\pm1})$
2.00E+02	0.272E-02	0.727E–01	0.420E-01	0.70154E–01
3.00E+02	0.376E-02	0.754E–01	0.419E-01	0.11799E–00
4.50E+02	0.718E-02	0.714E–01	0.498E-01	0.15281E–00
6.00E+02	0.159E-01	0.112E–00	0.741E-01	0.34763E–00
7.00E+02	0.196E-01	0.119E–00	0.143E-00	0.75897E–00
8.00E+02	0.194E-01	0.112E–00	0.179E-00	0.97687E–00
1.00E+03	0.145E-01	0.999E–01	0.668E-01	0.35843E–00
1.20E+03	0.136E-01	0.195E–00	0.866E-01	0.52813E–00
1.50E+03	0.138E-01	0.499E–00	0.162E-00	0.10379E+01
1.75E+03	0.157E-01	0.625E–00	0.479E-00	0.18749E+01
2.00E+03	0.183E-01	0.655E–00	0.727E-00	0.25187E+01
2.25E+03	0.199E-01	0.456E–00	0.870E-00	0.28696E+01
2.40E+03	0.204E-01	0.373E–00	0.925E-00	0.31031E+01
2.60E+03	0.170E-01	0.195E+01	0.835E-00	0.33901E+01
2.80E+03	0.138E-01	0.276E+01	0.925E-00	0.42142E+01
3.00E+03	0.116E-01	0.361E+01	0.918E-00	0.43270E+01

The calculated total SEC, DEC and excitation cross sections for ion-ion collisions He^{2+} – C^{4+}, N^{5+}, O^{6+} may be used in modeling of alpha-particles in thermonuclear plasma and in the design of future experiments.

All results presented above were obtained using our program package [7] for theoretical study of inelastic collisions.

Table 2. The total SEC+TE and dec cross sections and the partial excitation cross sections of $N^{5+}(1s^2)$ ion in $He^{2+} - N^{5+}$ collision

E (keV)	SEC+TE (10^{-16} cm^2)	DEC (10^{-20} cm^2)	$N^{5+}(1s2p_0)$ (10^{-16} cm^2)	$N^{5+}(1s2p_{\pm1})$
2.00E+01	0.534E-03	0.217E-03	0.496E-00	0.233E–00
1.00E+02	0.898E-03	0.181E-02	0.405E-00	0.265E–00
3.00E+02	0.128E-02	0.415E-02	0.212E-00	0.190E–00
5.00E+02	0.237E-02	0.544E-02	0.962E-01	0.124E–00
8.00E+02	0.444E-02	0.710E-02	0.112E-00	0.624E–01
1.00E+03	0.651E-02	0.904E-02	0.142E-00	0.738E–01
1.50E+03	0.535E-02	0.178E-01	0.241E-00	0.178E–00
2.00E+03	0.627E-02	0.303E-01	0.357E-00	0.373E–00
2.50E+03	0.597E-02	0.795E-01	0.481E-00	0.561E–00
3.00E+03	0.439E-02	0.170E-00	0.458E-00	0.938E–00
3.50E+03	0.391E-02	0.250E-00	0.679E-00	0.141E+01
3.80E+03	0.413E-02	0.261E-00	0.498E-00	0.133E+01
3.90E+03	0.430E-02	0.255E-00	0.516E-00	0.106E+01
4.00E+03	0.465E-02	0.247E-00	0.509E-00	0.905E–00
4.20E+03	0.571E-02	0.226E-00	0.458E-00	0.753E–00

Table 3. The total SEC+TE and DEC cross sections and the partial excitation cross sections of $O^{6+}(1s^2)$ ion in $He^{2+} - O^{6+}$ collision

E (keV)	SEC+TE (10^{-16} cm^2)	DEC (10^{-20} cm^2)	$O^{6+}(1s2p_0)$ (10^{-16} cm^2)	$O^{6+}(1s2p_{\pm1})$
3.00E+01	0.719E-03	0.300E-05	0.181E-00	0.101E–00
5.00E+01	0.838E-03	0.249E-05	0.204E-00	0.105E–00
1.00E+02	0.990E-03	0.209E-05	0.316E-00	0.132E–00
2.00E+02	0.127E-02	0.148E-05	0.353E-00	0.176E–00
4.00E+02	0.844E-03	0.684E-05	0.364E-00	0.235E–00
6.00E+02	0.619E-03	0.146E-04	0.234E-00	0.131E–00
1.00E+03	0.972E-03	0.460E-03	0.124E-00	0.804E–01
1.50E+03	0.185E-02	0.129E-02	0.799E-01	0.865E–01
2.00E+03	0.257E-02	0.300E-02	0.195E-00	0.263E–00
3.00E+03	0.284E-02	0.192E-01	0.212E-00	0.386E–00
4.00E+03	0.206E-02	0.632E-01	0.258E-00	0.611E–00
5.00E+03	0.165E-02	0.908E-01	0.453E-00	0.116E+01

This work was supported by IAEA (Research Contract N100088), by RFBR (project 99–02–17970) and by INTAS (Ref. N99–1326).

REFERENCES

[1] V.K. NIKULIN, N.A. GUSCHINA, J. Phys. B: Atom. Mol. Phys. **11** (1978) 3553.

[2] V.K. NIKULIN, N.A. GUSCHINA, Physica Scripta T **71** (1997) 134 .

[3] V.K. NIKULIN, N.A. GUSCHINA, "Two-electron description of excitation and charge-transfer in ion-ion He^{2+} – C^{4+}, N^{5+}, O^{6+} collisions". Preprint of Ioffe Physical-Technical Institute N 1740, St. Petersburg, 2000, 27 p.

[4] V.K. NIKULIN, N.A. GUSCHINA, "Electron Capture and Excitation in Ion-Ion Collision of Alpha Particles with He-like HCI". X Int. Conf. on the Physics of Highly Charged Ions, Book of Abstracts, Berkley 2000.

[5] M. RODBRO, E.H. PEDERSEN, C.L. COCKE, et al., Phys. Rev. A **19**, (1979) 1936.

[6] YU RANG KUANG, J. Phys. B: At. Mol. Opt. Phys. **25**, (1992) 199.

[7] N.A. GUSCHINA and V.K. NIKULIN. "The program package for inelastic process computation in slow ion–atom collisions". Preprint of Ioffe Physical-Technical Institute N 1717, St. Petersburg, 1998, 66 p.