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CALCULATION OF DEGRADATION SPECTRUM OF LOW ENERGY ELECTRONS WITHIN INFINITE HOMOGENEOUS BERYLLIUM OXIDE ON THE BASIS OF MATHEMATICAL MODELLING

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Abstract: Radiation-chemical yields of electron-ion pair $BeO_i^+ - e^-$ formed from direct onefold ionization of the products -different electron-excitation states ($1^1\Pi$ (V), $2\ ^1\Sigma^+$ (V), $1^1\Delta$ (V), $2\ ^1\Pi$ (V), $3\ ^1\Pi$ (R), $4\ ^1\Pi$ (R), $3\ ^1\Sigma^+$ (R), $2^1\Delta$ (R), $2\ ^1\Sigma^-$ (V), $2\ ^1\Sigma^-$ (R)) and different molecular orbital (O (1s), Be (1s), O (2s), Be (2s), O (2p)) of non-elastic collision between BeO molecules and low energy electrons (E= 1.0, 2.5, 5.0, 7.5 and 10.0 keV) have been calculated by mathematical modeling on the basis of Mathcad program using onefold collision, stepping, Monte-Carlo methods. Initial electrons and their new-generationδ-electrons lose some of their energy in each non-elastic collision and this process has been continued until the energy of all generation electrons creates non-elastic collision again. It has been used differential equationof 'dependence of effective cross section of collision on transmitted energy', which corresponds to the experimental values in these systems and suggested by Gryzinski for electron-electron interaction.

Key words: non-elastic collision, molecular orbital, electron-excitation state, onefold ionization

1. Introduction

Predicting the changes that may occur inside, on the surface and in a surrounding environment ofberyllium [1,2] and its different compounds (BeO, BeF_2, etc.)used as a construction material in atomic, nuclear and thermonuclear reactors by the influence of ionizing rays (γ-quanta, electrons, protons, neutrons, α-particles, etc.), has remained one of the main problems of researchers. Ionizing rays gradually lose their kinetic energies in elastic and non-elastic collision with atoms or molecules that form it,while passing through the substance. Non-elastic collision products contain different electron-excitation states, different type radiation defects, positive ion obtained from ionization and new generation electrons. New generation electrons [3-5] contain low (0.05÷10keV), medium (10÷100 keV) and high (100÷1000 keV) energy electrons and create a large spectrum. Those electrons gradually lose their kinetic energies in elastic and non-elastic collision with substance molecules (atoms) while passing through the substance.According to the mechanism of radiation loss of the energy, the active intermediate particles like electron-ion pair formed from direct onefold ionization of different orbital and electron excitation states are generated at the expense of the decrease of kinetic energy of initial electrons and their each new generation δ-electrons within non-elastic collision in the physical stage of the process ($10^{-15} \div 10^{-12}$ sec).Those active intermediate particles play an important role in the changeoccurred inside of substance, in the surrounding environment and substance-media border.

In the presented work, radiation-chemical yields of products (electron-ion pair formed from direct onefold ionization of various molecular orbital ***(O (1s), Be (1s), O (2s), Be (2s), O (2p))*** and various electron-excitation states***(1 $^1\Pi$ (V), 2 $^1\Sigma^+$ (V), $1^1\Delta$ (V), 2 $^1\Pi$ (V), 3 $^1\Pi$ (R), 4 $^1\Pi$ (R), 3 $^1\Sigma^+$ (R), $2^1\Delta$ (R), 2 $^1\Sigma^-$ (V), 2 $^1\Sigma^-$ (R))***) of non-elastic collision between BeO molecules and low energy *(E=1.0, 2.5, 5.0, 7.5 and 10.0 keV)* electrons have been calculated by mathematically modelling. It has been used differential equation of 'dependence of effective cross section on absorption energy', suggested by Gryzinski [6] for effective cross section of ionization and electron-excitation states in non-elastic collision. The calculation has been conducted using Monte-Carlo, onefold collision and stepping methods on the basis of Mathcad program.

2. Experimental part

We can express the energy balance in non-elastic collision between low-energy electrons and beryllium oxide moleculesin the following simplest way (1):

$$E = E_k + \Delta E \tag{1}$$

Here, E – is a kinetic energy of initial electron before collision, E_K –kinetic energy ofscattered orejected electron after collision, ΔE–the energy transmitted to beryllium oxide molecule by initial electron during collision. This energy is spent on different electron-excitation of beryllium oxide molecule (2):

$$e_0 + BeO \rightarrow BeO^*_{0,i} + e_s \left(\Delta E = E_{0,i}\right) \tag{2}$$

and direct onefold ionization of different orbital (3):

$$e_0 + BeO \rightarrow BeO^+_j + e_s + e_e \left(\Delta E = E_K + B_j\right) \tag{3}$$

Here, e_0, e_s, e_e - are initial, scattered, ejected electrons, respectively, BeO^+_j – onefold ionization of j^{th} orbital of beryllium oxide molecule and $BeO^*_{0,i}$ – i^{th} electron-excitation states. If we consider beryllium oxide molecule to be immobile before and after collision, the transmitted energy (ΔE) during these processes is equal to i^{th} electron-excitation energy in the state (2) and to the sum of kinetic energy (E_K) of ejected electron from j^{th} orbital and bonding energy (B_j) of corresponding orbital in the state (3).The transmitted energy ΔE can vary within the range of $\Delta E_{\min} = B_i$, $\Delta E_{\max} = \frac{E + B_i}{2}$ according to the law of energy and impulse maintenance in the process of ionization. The kinetic energy of ejected electrons can be defined by the expression (4):

$$E_K = \Delta E - B_j \tag{4}$$

It has been used differential equation of 'dependence of effective cross section on absorption energy [6]', suggested by Gryzinski for the calculation of effective cross section of non-elastic collision (the process of different electron-excitation and direct onefold ionization of orbital):

$$\frac{d\sigma_{i,j}(\Delta E, E, B_{i,j})}{d\Delta E} = \frac{\pi e^4}{\Delta E^3}\frac{B_{i,j}}{E}\left(\frac{E}{E + B_{i,j}}\right)^{\frac{3}{2}}\left(1 - \frac{\Delta E}{E}\right)^{\frac{B_{i,j}}{B_{i,j}+\Delta E}}\left\{\frac{\Delta E}{B_{i,j}}\left(1 - \frac{B_{i,j}}{E}\right) + \frac{4}{3}\ln\left[2.7 + \left(\frac{E - \Delta E}{B_{i,j}}\right)^{\frac{1}{2}}\right]\right\} \tag{5}$$

Here, e – is acharge of electron, $B_{i,j}$is equal to onefold ionization energyof j^{th} molecular orbital ($B_{i,j} = B_j$) in the ionization process, and to i^{th} electron-excitation energy($B_{i,j} = E_{0,i}$)in the electron-excitation state. It has been given the ionization energy [7] of beryllium oxide molecule corresponding different orbital - ***O(1s), Be(1s), O(2s), Be(2s), O(2p)*** in the table 1 and the excitation energy [8,9] corresponding to different electron-excitation - ***$1\,^1\Pi$ (V), $2\,^1\Sigma^+$ (V), $1^1\Delta$ (V), $2\,^1\Pi$ (V), $3\,^1\Pi$ (R), $4\,^1\Pi$ (R), $3\,^1\Sigma^+$ (R), $2^1\Delta$ (R), $2\,^1\Sigma$ (V), $2\,^1\Sigma$ (R)*** in the table 2.

If we integrate the expression (5), the differential equation corresponding to j^{th} orbital

according to all the possible values of transmitted energy ie. from $\Delta E_{\min}$ to $\Delta E_{\max}$ and multiply the obtained result by the number of electrons in the molecular orbital, we get the expression of dependence of effective cross section of ionization of that orbital on the kinetic energy of initial electron.

$$\sigma_j(E,B_j) = n_j \cdot \int_{\Delta E_{\min}}^{\Delta E_{\max}} \frac{d\sigma_j(\Delta E,E,B_j)}{d\Delta E} d\Delta E \tag{6}$$

In the figure 1, the graph of dependence of effective cross section of direct onefold ionization corresponding to j^{th}molecular orbital (***O(1s), Be(1s), O(2s), Be(2s), O(2p)***) of beryllium oxide molecule by the influence of low energy electrons, on its kinetic energy has been given on the basis of expression (6)

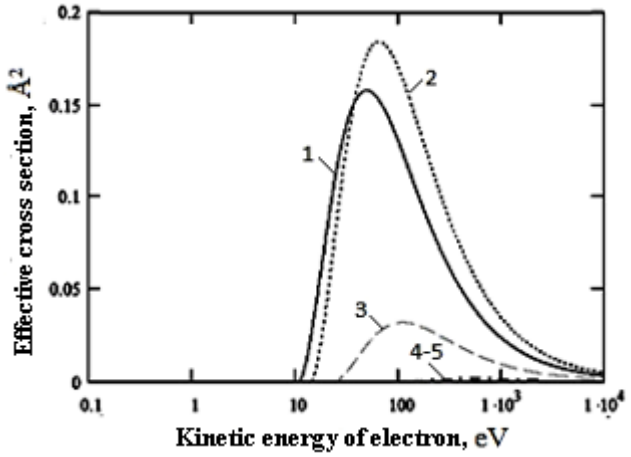

Fig.1. Dependence of effective cross section of direct one fold ionization corresponding to molecular orbital 1-Be(2s), 2-O(2p), 3-O(2s), 4-Be(1s), 5-O(1s) of beryllium oxide molecule by the influence of low energy electrons, on its kinetic energy

We should integrate the expression (5) for the width of peak (between two neighboring electron- excitement levels) in order to find effective cross section of the transition of electron from main state (*0)* to the i^{th}excitation state during non-elastic collision between low energy electrons and beryllium oxide.

$$\sigma_i(E,E_i) = \int_{E_i}^{E_{i+1}} \frac{d\sigma_i(\Delta E,E,E_{0i})}{d\Delta E} d\Delta E \tag{7}$$

Here, E_{0i} and E_{i+1} are i^{th} and $(i+1)^{th}$ electron-excitation energy, respectively. The graph of dependence of effective cross section of different electron-excitation states on the kinetic energy of electron has been given in the figure 2 on the basis of equation (8).

When we sum up the effective cross sections(6) of ionization, corresponding to different orbital we get fully effective cross section of ionization (figure 3 (2)):

$$\sigma_i(E) = \sum_j \sigma_j\left(E,B_j\right) \tag{8}$$

But when we sum up the effective cross sections (8) of different electron-excitation (exciton levels) we get fully effective cross section [10-12] of electron-excitation states (figure 3 (1)) [11,12]:

$$\sigma_i(E) = \sum_i \sigma_i\left(E, B_i\right) \tag{9}$$

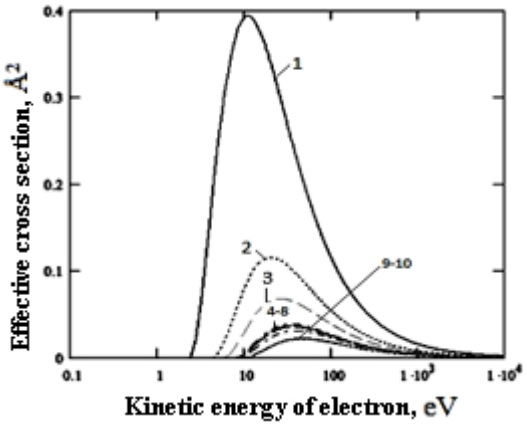

Fig. 2. Dependence of effective cross sections of electron-excitation (1-1 $^1\Pi$ (V), 2-2 $^1\Sigma^+$ (V), 3-1$^1\Delta$ (V), 4-2 $^1\Pi$ (V), 5-3 $^1\Pi$ (R), 6-4 $^1\Pi$ (R),7- 3 $^1\Sigma^+$ (R), 8-2$^1\Delta$ (R), 9-2 $^1\Sigma$ (V), 10-2 $^1\Sigma$ (R)) states generated inside BeO by the influence of low-energy electrons on its kinetic energy.

The sum of fully effective cross sections of ionization and electron-excitation states gives us the following fully effective cross section (figure 3 (3)):

$$\sigma_{tot}(E) = \sigma_j(E) + \sigma_i(E)$$

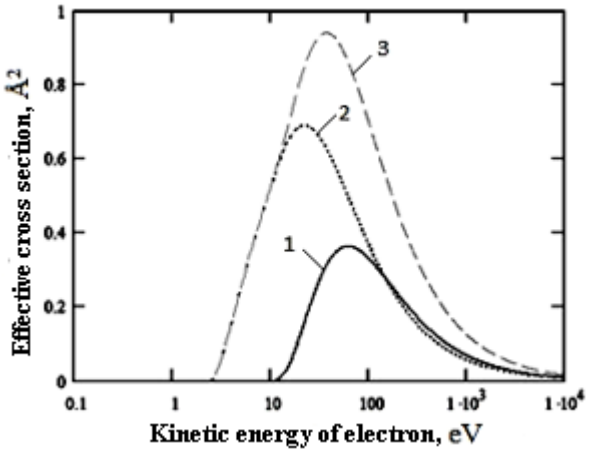

Fig. 3.The dependence of fully effective cross sections of the products - electron-excitation (1-σ_j(E)), *ionization* (2-σ_i(E)) *states of non-elastic collision between low energy electrons and beryllium oxide molecule and of their sum* $\sigma_{tot}(E) = \sigma_i(E) + \sigma_i(E)$ (3) *on the kinetic energy of electron.*

Initial electrons or their new generation δ-electrons lose certain part of their energy in each non-elastic collision and this process has been continued until the energy of electron forms non-elastic collision again. Amount of average energy $\Delta E(E)$, which is lost during each actin non-elastic collision with BeO molecules and the electron with the energy $E$is equal to the following expression [11,12]:

$$\Delta E(E) = \sum_i P_i(E) E_i + \sum_j P_j(E) \varepsilon_j(E) \tag{10}$$

Here, $P_i(E) = \dfrac{\sigma_i(E)}{\sigma_{tot}(E)}$ is probability of the transition of BeO molecule to i^{th} excitation state,

$P_j(E) = \frac{\sigma_j(E)}{\sigma_{tot}(E)}$ - of the occurrence ofcases corresponding to the ionization of the j^{th} orbital. $\varepsilon_j(E)$ is the average energy of the electron with the kinetic energy *E*for the formation of one electron-ion pair in j^{th}orbital.

$$\varepsilon_j(E) = \int_{Bj}^{E} \Delta E \frac{d\sigma_i(E)}{d\Delta E} d\Delta E$$

3. Results and Discussion

Low energy electrons become thermal electrons gradually losing their kinetic energy in elastic and non-elastic collision with beryllium oxide molecules. Radiation chemical yields products of non-elastic collision in the physical stage of the process - $BeO_i^+ - e^-$ – electron-ion pair and electron-excitation states***(1 $^1\Pi$ (V), 2 $^1\Sigma^+$ (V), $1^1\Delta$ (V), 2 $^1\Pi$ (V), 3 $^1\Pi$ (R), 4 $^1\Pi$ (R), 3 $^1\Sigma^+$ (R), $2^1\Delta$ (R), 2 $^1\Sigma$ (V), 2 $^1\Sigma$ (R))***formed as a result of onefold ionization of different orbital have been calculated on the basis of mathematical model.

The values obtained from calculation on the basis of model for the radiation chemical yields of electron-ion pair $(BeO_i^+ - e^-)$ formed from direct onefold ionization of different orbital (***O(1s), Be(1s), O(2s), Be(2s), O(2p))*** of beryllium oxide molecules by the influence of low energy electrons have been given in the table 1.

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Table l. *Radiation chemical yields of electron-ion pair* $(BeO_i^+ - e^-)$ *formed from direct one fold ionization of different orbital (O(1s), Be(1s), O(2s), Be(2s), O(2p)) of beryllium oxide molecules by the influence of low energy electrons*

Levels	Symbols	Number of electrons, n_i	Ionization energy, U_i, eV	Electron energy, keV				
				1	2,5	5	7,5	10
L-III	*Be(2s)*	2	11.0	1.765	1.663	1.589	1.552	1.903
M-I	*O(2p)*	4	13.6	2.489	2.41	2.328	2.285	1.826
L-II	*O(2s)*	2	24.4	0.613	0.633	0.628	0.623	0.734
K	*Be(1s)*	2	114.2	0.052	0.079	0.092	0.097	0.119
K	*O(1s)*	2	532.1	$5.291\cdot10^{-4}$	$4.287\cdot10^{-3}$	$8.432\cdot10^{-3}$	1.011	1.014

The values obtained from calculations on the basis of modelfor the radiation-chemical yields of different electron-excitation states***(1 $^1\Pi$ (V), 2 $^1\Sigma^+$ (V), $1^1\Delta$ (V), 2 $^1\Pi$ (V), 3 $^1\Pi$ (R), 4 $^1\Pi$ (R), 3 $^1\Sigma^+$ (R), $2^1\Delta$ (R), 2 $^1\Sigma$ (V), 2 $^1\Sigma$ (R))*** generated inside beryllium oxide by the influence of low energy electrons have been given in the table 2.

From the calculation based on model we come to the conclusion that, the radiation chemical yields of the products of non-elastic collision between low energy electron *(E=1.0, 2.5, 5.0, 7.5 and 10.0 keV*) and beryllium oxide molecules get the values of $G(BeO^+)=G(e^-)=3.66\div4.51$ electron-ion pair/(100 eV) forelectron-ion pair and $G(BeO^*)=14.5\div7.85$ excitation state/(100 eV) for electron excitation states depending on the energy of electron.

There is a clear correlation between the radiation chemical yields of active intermediate products (electron-hole pair obtained from direct onefold ionization of different electron-excitation states and orbital) calculated on the basis of our model in the physical stages ($10^{-15}\div10^{-12}$ sec) of processby the influence of low energy electrons and the different authors' results obtained from different theoretical calculations and experiments.

It is possible to calculate the amount of current density formed inside of substance by the influence of ionization rays, the amount of additional dose of substances adsorbed on the surface,

the amount of additional energy transmitted from BeO to the surrounding environment and the type of absorbed energy using this program. The calculation can be applied to practice.

Table 2. *Radiation-chemical yield of different electron-excitation states (1 $^1\Pi$ (V), 2 $^1\Sigma^+$ (V), 1$^1\Delta$ (V), 2 $^1\Pi$ (V), 3 $^1\Pi$ (R), 4 $^1\Pi$ (R), 3 $^1\Sigma^+$ (R), 2$^1\Delta$ (R), 2 $^1\Sigma^-$ (V), 2 $^1\Sigma^-$ (R)) generated within beryllium oxide by the influence of low energy electrons*

Excitation states	Excitation Energy-E_i, eV	Electron energy, keV				
		1	2,5	5	7,5	10
1 $^1\Pi$ (V)	2,46	3,492	2.979	2.748	2.638	2.584
2 $^1\Sigma^+$ (V)	4.55	0.973	0.851	0.794	0.767	0.754
1 $^1\Delta$ (V)	5.98	0.697	0.618	0.58	0.562	0.553
2$^1\Pi$ (V)	7.85	0.035	0.031	0.029	0.029	0.028
3 $^1\Pi$ (R)	7.97	0.033	0.03	0.029	0.028	$1.85\cdot10^{-4}$
4 $^1\Pi$ (R)	8.09	0.022	0.02	0.019	0.018	$1.204\cdot10^{-4}$
3$^1\Sigma^+$ (R)	8.17	0.138	0.124	0.118	0.114	0.113
2 $^1\Delta$ (R)	8.73	0.302	0.274	0.259	0.253	$1.684\cdot10^{-3}$
1 $^1\Sigma^-$(V)	10.38	0.025	0.023	0.022	0.021	0.211
2 $^1\Sigma^-$(R)	10,54	0.066	0.061	0.058	0.056	$3.782\cdot10^{-4}$

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ВЫЧИСЛЕНИЕ СПЕКТРА ДЕГРАДАЦИИ НИЗКОЭНЕРГЕТИЧЕСКИХ ЭЛЕКТРОНОВ В СОСТАВЕ ОДНОРОДНОГО ОКСИДА БЕРИЛЛИЯ ПУТЕМ МАТЕМАТИЧЕСКОГО МОДЕЛИРОВАНИЯ

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Резюме: С помощью математического моделирования в программе Mathcad, используя методы однократного столкновения, пошаговый и Монте-Карло, вычислены радиационно-химические выходы продуктов неупругих столкновений молекул BeO с низкоэнергетическими (E= 1.0, 2.5, 5.0, 7.5 и 10кэВ) электронами – различных электронно-возбужденных состояний (*(1$^1\Pi$ (V), 2 $^1\Sigma^+$ (V), 1$^1\Delta$ (V), 2 $^1\Pi$ (V), 3 $^1\Pi$ (R), 4 $^1\Pi$ (R), 3 $^1\Sigma^+$ (R), 2$^1\Delta$ (R), 2 $^1\Sigma^-$ (V), 2 $^1\Sigma^-$ (R))*), а также электрон-ионных пар

BeO^{*}-e^{-}, образованных прямой однократной ионизацией различных молекулярных орбиталей *(O (1s), Be (1s), O (2s), Be (2s), O (2p))*. Т.к. первичные электроны и созданные ими δ-электроны нового поколения теряют часть своей энергии при каждом неупругом столкновении, то вычисления были проведены до тех пор, пока энергии электронов всех поколений позволяют создавать неупругие столкновения. Было использовано дифференциальное уравнение, предложенное Гризинским для электрон-электронного взаимодействия и выражающее зависимость эффективного поперечного сечения от энергии, экспериментально подтвержденную для данных систем.

Ключевые слова: неупругое столкновение, молекулярная орбиталь, электронно-возбужденное состояние, однократная ионизация.

KİÇİK ENERJİLİ ELEKTRONLARIN SONSUZ BİRCİNS BERİLLİUM OKSİD DAXİLİNDƏ DEQRADASİYA SPEKTRİNİN RİYAZİ MODEL ƏSASINDA HESABLANMASI

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Xülasə: Birqat toqquşma, addımlama və Monte-Karlo metodlarından istifadə edərək **Mathcad** proqramı əsasında BeO molekulları ilə kiçik enerjili elektronlar (E=1.0, 2.5, 5.0, 7.5 və 10.0 keV) arasında qeyri-elastiki toqquşma məhsulları-müxtəlif elektron-həyacanlanma hallarının ($1^1\Pi$ (V), $2\ ^1\Sigma^+$ (V), $1^1\Delta$ (V), $2\ ^1\Pi$ (V), $3\ ^1\Pi$ (R), $4\ ^1\Pi$ (R), $3\ ^1\Sigma^+$ (R), $2^1\Delta$ (R), $2\ ^1\Sigma^-$ (V), $2\ ^1\Sigma^-$ (R)) və müxtəlif molekulyar orbitalların (O (1s), Be (1s), O (2s), Be (2s), O (2p)) birbaşa birqat ionlaşmasından əmələgələn elektron-ion cütünün $BeO_i^+ - e^-$ radiasiya-kimyəvi çıxımları riyazi modelləşdirilərək hesablanmışdır. Hesablama, ilkin electronlar və onların yaratdıqları yeni nəsil δ-elektronlar hər bir qeyri-elastiki toqquşmada özlərinin enerjilərinin müəyyən hissəsini itirirlərki, bu proses bütün nəsil elektronların enerjisinin yenidən qeyri-elastiki toqquşma yarada bilənə kimi davam etdirilmişdir. Elektron-elektron qarşılıqlı təsiri üçün Qrizinskinin təklif etdiyi və bu sistemlərdə təcrübi qiymətlərlə uyğunlaşan toqquşmanın effektiv en kəsiyinin ötürülən enerjidən asılılığı, differensial tənliyindən istifadə edilmişdir.

Açar sözlər: qeyri elastiki toqquşma, molekulyar orbital, electron həyəcanlanma halı, birqat ionlaşma