International Journal of Mass Spectrometry 372 (2014) 8–12

Contents lists available at ScienceDirect

International Journal of Mass Spectrometry

journal homepage: www.elsevier.com/locate/ijms

Calculation of electron impact total ionization cross sections for tungsten, uranium and their oxide radicals

Biplab Goswami, Rahla Naghma, Bobby Antony *

Department of Applied Physics, Indian School of Mines, Dhanbad 826004, Jharkhand,India

ARTICLE INFO

Article history:
Received 1 June 2014
Received in revised form 9 August 2014
Accepted 9 August 2014
Available online 17 August 2014

Keywords:
Electron impact ionization
Total ionization cross section
SCOP
CSP-ic
WO_x
UO_x

ABSTRACT

The present article reports total ionization cross section for W, WO, WO_2, WO_3, U, UO, UO_2 and UO_3 targets by electron impact. Tungsten is used as a wall coating element in fusion reactors and are found as impurities in the fusion edge plasma along with their oxides. Uranium and its oxides are found especially in nuclear reactors. In both cases, electron induced collision and ionization are the most probable reaction that can take place in such environments. Hence, the knowledge of electron impact cross section data is very important for the modelling of these reactors. The total inelastic cross sections for these targets were calculated using spherical complex optical potential (SCOP) formalism. Then by employing complex scattering potential ionization contribution (CSP-ic) method, total ionization cross sections is derived from inelastic cross section. The present results show reasonable agreement with previous theories and experiments, wherever available. A linear relation between the ionization potential and peak of ionization cross section was also obtained confirming the consistency of the data reported here. The total ionization cross sections for UO, UO_2 and UO_3 presented in this work is reported for the first time.

1. Introduction

Atomic tungsten (W) and their oxides radicals (WO, WO_2 and WO_3) are the main atomic and molecular impurities at edge plasma in fusion reactors [1]. W is also used in wall coating inside magnetic fusion devices such as tokamak due to its low sputtering rates. On the other hand, uranium is a common nuclear fuel. The relativistic effects and bonding nature of the *f* valance orbital electrons in ionization processes for uranium oxides clusters has ignited clear attention [2]. It is also used in radio-therapy for ionizing radiation to kill cancer cells [3]. Uranium reacts strongly with oxygen and produces various oxides due to strong electro-positive behaviour. These uranium oxides can be used primarily as nuclear fuel in the form of fuel rods in nuclear reactor [4]. The low thermal conductivity of UO_2 compared with uranium nitride or uranium carbide can result in restricting overheating particularly at the centre of the fuel plates [5]. All the above mentioned environments are electron rich and hence, the most likely reaction channel will be electron induced collision and ionization of the molecules present. Consequently, the necessity of electron induced ionization cross section for tungsten, uranium and their oxides are vital, particularly for modelling fusion and nuclear reactors having electron rich gaseous medium.

Despite these applications, only few attempts have been made to obtain electron impact ionization cross sections for these targets. Deutsch et al. [6] calculated total ionization cross sections by electron impact for W, WO, WO_2 and WO_3 targets using Deutsch–Märk (DM) formalism and modified additivity rule. Halle et al. [7] measured total electron impact ionization cross section for U atom using modulated crossed-beam experiment. They measured the ion number cross sections (Q_{ion}) of U from the total current produced. They have also determined the electron production cross section (Q_e) from the charge weighted in the scattering system [7]. Calculation on electron impact ionization cross section was also done by Mann [8] by utilizing a method of summation with the mean-square orbital radii of outer electrons. There are no previous results reported in the literature for electron impact total ionization cross section for uranium oxides. In this article, we have reported total ionization cross sections by electron impact for the above mentioned targets from ionization threshold to 5000 eV. The methodology adopted here has been successfully used to evaluate the ionization cross sections for a large number of targets [10–17]. The reliability of the data obtained for various targets using the SCOP and CSP-ic methods has encouraged us to report the ionization cross sections for these less studied species. The theoretical methodology employed here for the calculations is discussed in the next section.

* Corresponding author. Tel.: +91 9470194795.
E-mail address: bka.ism@gmail.com (B. Antony).

http://dx.doi.org/10.1016/j.ijms.2014.08.018
1387-3806/

2. Theoretical methodology

A brief outline of the theory to calculate total ionization cross section for these atoms and their oxides is given in this section. The total inelastic cross sections are calculated using a quantum mechanical approach called spherical complex optical potential (SCOP) formalism [9,10]. Then the ionization cross section is derived from the inelastic cross section by applying the complex scattering potential ionization contribution (CSP-ic) method [10–17]. Detailed theoretical methodology is explained in our previous articles [9–17].

In SCOP formalism, a complex potential is formulated and incorporated in the Schrödinger equation. Then partial wave analysis as used to obtain the solution for the asymptotic wave function from Schrödinger's equation [18]. This solution contains complex phase shifts that represent the complete information regarding electron scattering with the target. The complex optical potential (V_{opt}) used in the calculation has the form,

$$V_{opt}(r, E_i) = V_R(r, E_i) + iV_I(r, E_i) \quad (1)$$

here the real potential is expressed as,

$$V_R(r, E_i) = V_{st}(r) + V_{ex}(r, E_i) + V_p(r, E_i) \quad (2)$$

and the imaginary potential is given by

$$V_I(r, E_i) = V_{abs}(r, E_i) \quad (3)$$

The energy of the incident electron is represented by E_i. The real term in Eq. (1) is the sum of static (V_{st}), exchange (V_{ex}) and polarization potential (V_{pol}) as expressed in Eq. (2). The imaginary part of Eq. (1) is the absorption potential, which considers the total loss of scattered flux into the allowed electronic excitation and ionization channels. For calculating all these potentials, the spherically averaged molecular charge density, $\rho(r)$ has to be determined. The molecular charge density is obtained using the atomic charge density derived from the parameterized relativistic Dirac Hartree–Fock wavefunction of Salvat et al. [19]. In the present calculations, the charge density for the radicals is obtained by adding up the charge densities of constituent atoms, as they are widely placed in the molecule. The wavefunctions reported by Salvat et al. [19] are used to calculate the static potential of the targets. The parameter free Hara's energy dependant 'free electron gas exchange model' [20] is employed for the exchange potential. The polarization potential is devised from the parameter free model of correlation-polarization potential given by Zhang et al. [21]. Here the non-spherical terms due to vibrational and rotational excitation of the target are neglected, since these processes are dominant mostly at low incident energies.

The well known, non-empirical and quasi-free model of Staszewska et al. [22] is used for the absorption potential. The expression for V_{abs} is given as,

$$V_{abs}(r, E_i) = -\rho(r)\sqrt{\frac{T_{loc}}{2}}\left(\frac{8\pi}{10k_F^3 E_i}\right)\theta\left(p^2 - k_F^2 - 2\Delta\right)(A_1 + A_2 + A_3) \quad (4)$$

The local kinetic energy of the incident electron is expressed as,

$$T_{loc} = E_i - (V_{st} + V_{ex}) \quad (5)$$

Here $p^2 = 2E_i$, $k_F = \left[3\pi^2\rho(r)\right]^{1/3}$ is the Fermi wave vector and A_1, A_2 and A_3 are dynamic functions that depends differently on $\theta(x)$, I, Δ and E_i. I is the ionization threshold of the target, $\theta(x)$ is the Heaviside unit step-function and Δ is an energy variant parameter below which $V_{abs} = 0$. Hence, Δ is the dominant factor which resolves the results of total inelastic cross section; since, below this value, ionization or excitation is not allowed. This is one of the main attribute of the original Staszewska model [22].

The phase shifts obtained using the partial wave analysis as the solution of Schrödinger equation are used to calculate inelastic and

Table 1
Parameters used in Eq. (10) to find $R(E_i)$ for the targets.

Molecules	Ionization potential (eV) [23]	a	C_1	C_2
W	7.98	6.736	−1.115	−6.940
WO	9.00	6.926	−1.104	−7.179
WO_2	9.50	7.213	−1.093	−7.511
WO_3	12.50	7.350	−1.090	−7.661
U	6.19405	6.698	−1.117	−6.891
UO	5.66	6.507	−1.134	−6.622
UO_2	5.40	6.625	−1.123	−6.791
UO_3	10.60	6.300	−1.162	−6.281

Table 2
Q_{ion} in Å^2 for the present targets.

Energy (eV)	W	WO	WO_2	WO_3	U	UO	UO_2	UO_3
6	–	–	–	–	–	–	0.03	–
7	–	–	–	–	0.06	0.22	0.40	–
8	–	–	–	–	0.43	0.84	1.20	–
9	0.02	–	–	–	1.08	1.74	2.23	–
10	0.12	0.01	–	–	1.89	2.75	3.34	–
11	0.31	0.08	0.03	–	2.76	3.77	4.42	–
12	0.58	0.21	0.11	–	3.62	4.74	5.41	0.03
13	0.90	0.39	0.24	–	4.43	5.61	6.29	0.12
14	1.24	0.62	0.42	0.01	5.17	6.38	7.05	0.27
15	1.59	0.87	0.63	0.04	5.83	7.05	7.70	0.47
16	1.93	1.14	0.85	0.10	6.40	7.62	8.26	0.72
17	2.27	1.41	1.09	0.18	6.90	8.11	8.73	0.99
18	2.58	1.67	1.32	0.27	7.33	8.53	9.12	1.28
19	2.88	1.93	1.56	0.39	7.70	8.88	9.45	1.56
20	3.15	2.18	1.79	0.51	8.02	9.17	9.73	1.85
22	3.64	2.64	2.22	0.77	8.51	9.62	10.15	2.40
24	4.04	3.04	2.61	1.04	8.85	9.93	10.44	2.90
26	4.37	3.38	2.95	1.31	9.09	10.13	10.63	3.34
28	4.64	3.68	3.25	1.56	9.25	10.27	10.75	3.73
30	4.86	3.93	3.51	1.80	9.35	10.35	10.82	4.06
32	5.03	4.14	3.74	2.02	9.40	10.39	10.86	4.35
34	5.17	4.32	3.93	2.22	9.43	10.40	10.87	4.60
36	5.28	4.47	4.10	2.40	9.43	10.39	10.85	4.81
38	5.36	4.59	4.24	2.56	9.42	10.36	10.83	4.99
40	5.43	4.70	4.36	2.71	9.39	10.32	10.79	5.14
42	5.48	4.79	4.47	2.84	9.35	10.27	10.74	5.28
44	5.52	4.86	4.56	2.96	9.30	10.22	10.69	5.39
46	5.54	4.92	4.63	3.07	9.25	10.16	10.63	5.48
48	5.56	4.97	4.70	3.17	9.20	10.10	10.57	5.56
50	5.57	5.01	4.76	3.26	9.14	10.03	10.50	5.63
55	5.57	5.07	4.86	3.44	8.99	9.86	10.33	5.75
60	5.55	5.11	4.93	3.58	8.83	9.69	10.16	5.83
65	5.51	5.12	4.97	3.68	8.67	9.52	9.99	5.87
70	5.46	5.11	4.98	3.77	8.52	9.35	9.83	5.89
75	5.41	5.09	4.99	3.83	8.37	9.19	9.66	5.89
80	5.35	5.07	4.98	3.87	8.22	9.04	9.51	5.88
85	5.29	5.03	4.97	3.90	8.08	8.88	9.36	5.86
90	5.23	5.00	4.95	3.93	7.95	8.74	9.21	5.83
95	5.17	4.96	4.92	3.94	7.82	8.60	9.07	5.80
100	5.10	4.92	4.90	3.95	7.69	8.47	8.93	5.76
110	4.99	4.83	4.83	3.95	7.45	8.21	8.68	5.68
120	4.87	4.74	4.76	3.94	7.24	7.98	8.44	5.59
130	4.76	4.66	4.69	3.91	7.03	7.76	8.22	5.50
140	4.66	4.57	4.62	3.89	6.84	7.56	8.01	5.41
150	4.56	4.49	4.55	3.85	6.67	7.37	7.82	5.32
200	4.13	4.12	4.22	3.66	5.94	6.58	7.01	4.91
250	3.79	3.82	3.93	3.46	5.39	5.99	6.39	4.56
500	2.79	2.87	3.01	2.73	3.85	4.29	4.57	3.45
1000	1.96	2.04	2.16	2.00	2.60	2.76	3.03	2.46
2000	1.32	1.39	1.48	1.38	1.64	1.95	2.16	1.67
3000	1.03	1.09	1.16	1.08	1.31	1.55	1.70	1.31
4000	0.86	0.91	0.97	0.90	1.09	1.29	1.44	1.09
5000	0.74	0.78	0.84	0.78	0.94	1.10	1.26	0.94