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International Journal of Mass Spectrometry 252 (2006) 213–221

International Journal of Mass Spectrometry

www.elsevier.com/locate/ijms

Ionization of W and W^+ by electron impact

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Received 19 January 2006; received in revised form 8 March 2006; accepted 8 March 2006
Available online 25 April 2006

Abstract

Theoretical cross-sections for electron-impact ionization of the neutral W atom and W^+ ion are reported. The direct ionization cross-sections were calculated by using the binary-encounter Bethe (BEB) model and the indirect ionization cross-sections resulting from numerous excitation-autoionization (EA) were calculated by using scaled Born cross-sections. Contributions to indirect ionization from spin-forbidden and $\Delta n = 1$ excitations, where n is the principal quantum number, are noticeable unlike in light atoms. The single ionization cross-section of W^+ is increased by about 10% due to the indirect EA of 5p electrons in the range of the incident electron energies between 40 and 60 eV. In the case of neutral W the EA cross-sections are very small for the $^7S_3$ level which is the first metastable term of W and because the excitations to the high spin states are mostly in the bound spectrum below the ionization limit. On the other hand, the EA cross-section of the second metastable ^3P term of W is large where a few $6s^2 \rightarrow 5d6p$ and many $5p \rightarrow 5d$, 6s excitations increase the total ionization cross-section by as much as 25%. Our total cross-section for the single ionization of W^+ is $\sim 15\%$ higher at the peak than the two sets of experimental data available in the literature. Our cross-sections are compared to the scaled Born cross-sections derived from the formulas provided by McGuire and those derived from the semi-empirical formulas by Lotz.
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Keywords: Ionization cross-section; W, W^+; Autoionization

1. Introduction

Electron-impact ionization of tungsten (W, atomic number $Z = 74$) and tungsten ions have been investigated by some authors [1–3] because tungsten is a refractory material which will be used inside magnetic fusion devices such as tokamak. In spite of strong radiative loss of high-Z tungsten, the ASDEX (Axially Symmetric Divertor Experiment) Upgrade tokamak in Germany is designed to use tungsten facing in the divertor region to take advantage of very low sputtering rates of tungsten similar to the ITER (International Thermonuclear Experimental Reactor) plan. Therefore, electron-impact ionization cross-sections of tungsten and tungsten ions are essential data for divertor modeling. The ionization cross-section of singly charged tungsten ion (W^+) by electron impact was experimentally measured by two different groups, Montague and Harrison [1] and Stenke et al. [2]. However, the electron-impact ionization cross-section of neutral tungsten could not be measured because of low vapor pressure owing to the high melting point. The cross-section of W^+ measured by Montague and Harrison [1] was compared to the scaled Born prediction of McGuire [4]. McGuire's calculation is in good agreement with the measurement at higher incident electron energies over 100 eV but it underestimates the cross-section at energies below 100 eV. On the other hand the measured cross-section of W^+ by Stenke et al. [2] is lower than the configuration-average, distorted-wave Born (DWB) cross-section by Pindzola and Griffin [3] and the one-term Lotz formula [5]. Electron-impact ionization cross-section of the neutral atom was also calculated by Pindzola and Griffin [3] near the threshold using the DWB approximation. Their result shows however very different shape and peak position compared to the cross-section from the one-term Lotz formula [5].

We report in this article ionization cross-sections of neutral W and W^+ ion using the binary-encounter Bethe (BEB) model [6] for direct ionization of all electrons and scaled Born cross-section [7,8] for excitation-autoionization (EA) of outer-shell electrons. These methods have successfully been applied to Mo ($Z = 42$) and Mo^+ [9], which have half-filled 4d valence shell

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1387-3806/$ – see front matter. Published by Elsevier B.V.
doi:10.1016/j.ijms.2006.03.007

similar to W and W^+, as well as to light atoms such as B ($Z = 5$), C ($Z = 6$), N ($Z = 7$), O ($Z = 8$), Al ($Z = 13$), Ga ($Z = 31$) and In ($Z = 49$) [10,11]. We calculated total ionization cross-sections of W and W^+ for ground, first and second metastable levels individually and compared our results with experiments and theories by McGuire [4] and Lotz [5,12,13].

2. Theoretical procedure

Open shell atoms have two dominant processes contributing to ionization. The first is direct ionization caused by the ejection of bound electrons to continuum states. The second is indirect ionization through excitation-autoionization (EA) of outer-shell electrons into quasi-bound states above the lowest ionization limit. We used binary-encounter Bethe (BEB) model [6] for the direct ionization. The BEB cross-section for the direct ionization of electrons in an atomic orbital is given by

$$\sigma_{\text{neut}}=\frac{4\pi a_0^2 NR^2}{B^2[t+(u+1)/m]}\left[\frac{\ln t}{2}\left(1-\frac{1}{t^2}\right)+1-\frac{1}{t}-\frac{\ln t}{t+1}\right], \tag{1}$$

for a neutral atom, and by

$$\sigma_{+}=\frac{4\pi a_0^2 NR^2}{B^2[t+(u+1)/2m]}\left[\frac{\ln t}{2}\left(1-\frac{1}{t^2}\right)+1-\frac{1}{t}-\frac{\ln t}{t+1}\right], \tag{2}$$

for a singly charged ion. In Eqs. (1) and (2), a_0 is the Bohr radius, N the orbital electron occupation number, R the Rydberg energy, B the orbital binding energy, $t = T/B$ with the incident electron energy T, and $u = U/B$ with the orbital kinetic energy U. The constant m in the denominator is unity for K- and L-shell orbitals, and m = principal quantum number n of other orbitals.

The first logarithmic term in Eqs. (1) and (2) came from the leading part of the Bethe cross-section, the middle term, $1 - 1/t$, from the direct and pure exchange part of the Mott cross-section, and the last logarithmic term from the interference between the direct and exchange terms of the Mott cross-section. The total direct ionization cross-section is obtained by summing σ over all occupied orbitals. The denominator, $t + u + 1$, is a modification of the original plane-wave Born (PWB) and Mott cross-sections to emulate the increased flux of the incident electron resulting from its interaction with the target atom. Most collision theories, including the original PWB and Mott cross-sections, have only t in the denominator.

The factor m was introduced to avoid unrealistically small cross-sections resulting from increasing values of U as n increases for outer orbitals in heavy atoms. The introduction of the factor 2 in the denominator of Eq. (2) reflects the fact that the original Mott cross-section with only t in the denominator will eventually become accurate for highly charged ion targets. Both modifications have successfully been applied to molecules and molecular ions that contain heavy atoms [14].

Note that Eqs. (1) and (2) require data only from the initial bound states, which are far easier to calculate than properties that directly involve continuum states. Besides, Eqs. (1) and (2) are based on nonrelativistic theories and hence valid only for nonrelativistic T. We obtained the atomic data B, U and N of the initial bound state of target W and W^+ using relativistic wave functions from a multiconfiguration Dirac-Fock (MCDF) code [15].

Excitation-autoionization cross-sections were obtained using scaled PWB cross-sections for the neutral W and scaled Coulomb Born (CB) cross-sections for W^+. The unscaled PWB and CB approximations are based on the first-order perturbation theory and are reliable only at high T. Moreover, these approximations do not account for the electron exchange effect with the bound electrons in the target atom, the distortion of plane or Coulomb waves in the vicinity of the target atom, or the polarization of the target atom due to the presence of the incident electron. Hence, we adopted simple scaling methods called *BE scaling* [7] for PWB cross-sections and *E scaling* [8] for CB cross-sections as was done in the case of Mo and Mo^+ [9]. These scalings offer simple ways to correct the deficiencies of the Born approximations. These scalings can be used to modify the Born cross-sections at low T so that they become reliable at all T. The BE scaling is given by

$$\sigma_{\text{BE}} = \sigma_{\text{PWB}}\frac{T}{T+B+E}, \tag{3}$$

and the E scaling by

$$\sigma_{\text{E}} = \sigma_{\text{CB}}\frac{T}{T+E}, \tag{4}$$

where E is the excitation energy. Both the BE scaling and the E scaling have been verified to produce reliable results at low T for light as well as heavy atoms [7,8] even though the BE and E scaling cannot be derived from first principles. These scaling methods can be used for excitations to both low-lying (hence true bound) levels as well as highly excited (i.e., autoionizing) levels. However these scalings are valid only for electric dipole ($E1$)-*allowed, strong* excitations and cannot be used for weak processes such as $E1$-forbidden excitations because cross-sections for such weak transitions cannot be accurately described by the first-order Born approximation, particularly at low T. We included $E1$-allowed ($\Delta J = 0, \pm 1$), strong transitions with the oscillator strength $f > 0.05$ among many transitions to autoionizing levels above the lowest ionization limit.

In the calculation of CB cross-sections for W^+, the incident electron before and after the collision is represented by partial waves. The cross-sections for high T far from excitation thresholds do not easily converge because of the large number of partial waves needed. In order to obtain cross-sections valid for the entire range of T, we combined high-T PWB cross-sections, which can be represented by the Bethe approximation with constants α, β, and γ [16]:

$$\sigma_{\text{Bethe}}(T) = \frac{4\pi a_0^2}{T/R}\left[\alpha \ln\left(\frac{T}{R}\right)+\beta+\frac{\gamma R}{T}\right], \tag{5}$$

with the CB cross-sections near the thresholds by using a least squares fit with a four term polynomial with fitting constants b,