Electron-impact ionization of the tungsten atom

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The near-threshold electron-impact ionization cross section for the tungsten atom is calculated in a distorted-wave approximation. A shape resonance is found to have a large effect on the total cross sections for the 6s and 5d subshells. The shape resonance in the $l=2$ scattering channel is most clearly defined when one examines the differential cross section with ejected energy.

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Electron-collision processes involving heavy atoms and their ions yield certain phenomena not found in lighter atomic systems. One of the more interesting features is the appearance of giant shape resonances in the electron-impact ionization cross section [1–5]. The theoretical studies have examined inner-shell 4d and 4f ionization cross sections along isoionic, isoelectronic, and isonuclear sequences of heavy atoms. The best experimental indication of the 4d shape resonance feature is found in double-ionization measurements of the I^+, Xe^+, and Cs^+ ions [6–8]. Shape resonances have also been found in valence subshell ionization calculations for Cs^+, La^+, and Ce^+ ions; in the case of La^+ there is a good indication of the resonance feature in single-ionization measurements [9]. In this paper we report on the occurrence of a strong shape resonance in calculations of the 6s and 5d valence subshell ionization cross sections for neutral W. Besides reporting integrated ionization cross sections, we also examine the differential cross section with ejected energy which most clearly defines the shape resonance feature. Although there has been a great deal of experimental work on the electron-impact ionization of atoms [10,11], measurements on W and its nearest neighbors in the Periodic Table are still lacking. Our original motivation for examining W is a revived interest in this highly refractory metal for use in future fusion reactors.

The direct-ionization cross section for an atomic subshell may be calculated using a configuration-average distorted-wave method [12]. The total ionization cross section (in atomic units) is given by

$$\sigma=\int_0^{E/2}\frac{d\sigma}{d\varepsilon_e}d\varepsilon_{e'}\ , \qquad (1)$$

where the differential cross section with ejected energy may be written

$$\frac{d\sigma}{d\varepsilon_e}=\frac{32q}{k_i^3k_ek_f}\sum_{l_i}\sum_{l_e}\sum_{l_f}(2l_i+1)(2l_e+1)(2l_f+1)\times|V(ef;bi)|^2_{\text{av}}\ . \qquad (2)$$

In Eqs. (1) and (2), $(\varepsilon_i,\varepsilon_e,\varepsilon_f)$ are the single-particle energies, (k_i,k_e,k_f) are the linear momenta, and (l_i,l_e,l_f) are the angular momenta of the initial, ejected, and final scattering partial waves, respectively. The energy $E=\varepsilon_e+\varepsilon_f=\varepsilon_i-I$, I is the subshell ionization potential, and q is the occupation number of the subshell. The continuum normalization is chosen as one times a sine function. As previously discussed [12], the configuration-average reduced matrix element squared $|V(ef;bi)|^2_{\text{av}}$, contains direct and exchange scattering terms and the interference between the two. The bound-state orbitals needed to evaluate the Slater radial integrals found in the reduced matrix element are calculated using a wave-function code developed by Cowan [13]. The code employs a Hartree-Fock method with relativistic modifications (HFR), which includes the mass-velocity and Darwin relativistic corrections within modified differential equations [14]. The continuum-state orbitals needed to evaluate the Slater integrals are obtained by solving the radial Schrödinger equation in the distorted-wave approximation. Although the major relativistic effect on the continuum orbitals is the relativistic modification of the target distorting potentials, mass-velocity and Darwin terms are also included in the distorted-wave equations.

The results of distorted-wave calculations for the differential cross section of the 6s, 5d, and 4f subshells of neutral W are shown in Fig. 1. The ground-state configuration of W is [Xe core]$4f^{14}5d^46s^2$. The subshell ionization potentials are $I_{6s}=7.61$ eV, $I_{5d}=8.37$ eV, and $I_{4f}=40.5$ eV. In each case the incident electron energy is 1.5 times the subshell ionization potential. Each differential cross section is dominated by a large shape resonance which peaks at about $E_{\text{res}}=1.37$ eV ejected energy. The resonance occurs in the $l=2$ final scattering channel, whose phase shift increases by almost π around the peak energy. As previously discussed [1–5], shape resonances occur in heavy atoms and ions which can support double- (or even triple-) potential-well structures.

In general the energy positions of resonance structures in the differential cross section change as a function of incident energy. For compound resonance structures, due to excitation of autoionizing states in the ejected scattering channel, Moores and Reed [15] have given a complete description of their changing energy positions. For shape resonance structures, which appear in the final scattering channel, three cases can be distinguished. (i) For $\varepsilon_i < I + E_{\rm res}$, the full resonance does not appear in the differential cross section. (ii) For $I + E_{\rm res} < \varepsilon_i < I + 2E_{\rm res}$, the full resonance appears in the direct scattering term and its peak in the differential cross section occurs at $\varepsilon_e = \varepsilon_i - I - E_{\rm res}$. As ε_i increases for this case the resonance appears to move from left to right. (iii) For $\varepsilon_i > I + 2E_{\rm res}$, the full resonance appears in the exchange scattering term and its peak in the differential cross section remains fixed at $\varepsilon_e = E_{\rm res}$. The cross sections shown in Fig. 1 represent this last case.

The results of distorted-wave calculations for the total cross section of the 6*s*, 5*d*, and 4*f* subshells of neutral W are shown in Fig. 2. The 6*s* and 5*d* subshell cross sections, which sum to give the bulk of the single-ionization cross section for W, both show a large resonance feature at 1.25 times threshold. The 4*f* subshell cross section, which should contribute to the double-ionization cross section for W, shows a resonance "knee" at 1.02 times threshold. The single-parameter Lotz formula [16] given by

$$\sigma(10^{-16}\ {\rm cm}^2) = \frac{450q\ \ln x}{xI^2}\ , \tag{3}$$

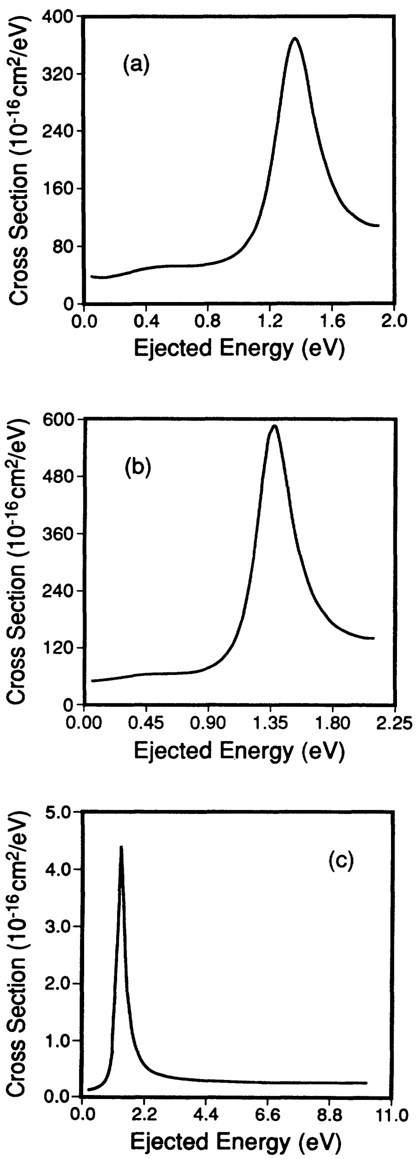

FIG. 1. Differential cross sections with ejected energy for the electron-impact ionization of neutral W. (a) 6*s* subshell; (b) 5*d* subshell; (c) 4*f* subshell. Incident energies are 1.5 times the corresponding subshell ionization potential.

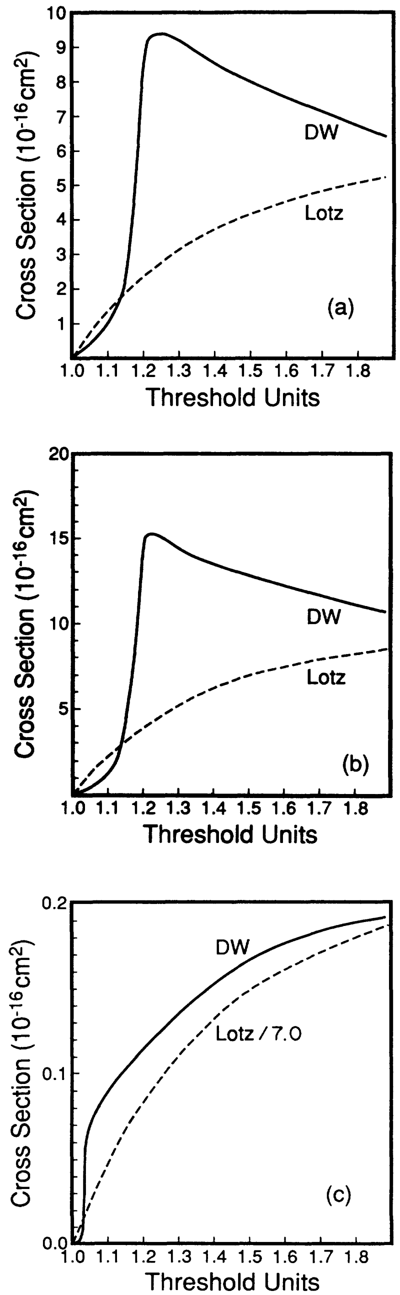

FIG. 2. Total cross sections for the electron-impact ionization of neutral W. (a) 6*s* subshell; (b) 5*d* subshell; (c) 4*f* subshell. Solid curves are distorted-wave results; dashed curves are from the Lotz formula. Threshold units are defined as incident energy divided by subshell ionization potential.

where x is the energy in threshold units and I is in eV, is used to draw the dashed curves for comparison in Fig. 2. The Lotz formula is widely used to estimate ionization cross sections for plasma modeling. The occupation number q is taken to be 2 for the $6s$ subshell and 4 for the $5d$ subshell, but is arbitrarily assigned 2 (instead of 14) for the $4f$ subshell to keep it on the graph.

We carried out several other configuration-average excitation and ionization calculations which relate to the giant shape resonance found in neutral W. First we found little qualitative difference between calculations carried out in the Hartree-Fock and HFR methods. Thus the shape resonance does not appear to be sensitive to small changes in the electrostatic potential. We also calculated $6s$ subshell ionization cross sections for the ground-state configuration of Ta and W^+, given by [Xe core]$4f^{14}5d^4 6s$. For Ta a large shape resonance was again found, but for W^+ no shape resonance appeared. As previously discussed [2,4,5], shape resonances disappear quite quickly along isoelectronic and isonuclear sequences. To assess the importance of excitation-autoionization contributions to the single-ionization cross section for W, we carried out several configuration-average calculations for excitation from inner subshells. No sizable contribution to the ionization process was found. Thus the sum of the direct-ionization cross sections for the $6s$ and $5d$ subshells should give the dominant contribution to the single-ionization cross section of neutral W.

To illustrate the quantitative accuracy expected from the distorted-wave ionization calculations for neutral W, we also computed direct-ionization cross sections for the $6s$ and $5d$ subshells of W^+. As shown in Fig. 3, the crossed-beams measurements of Montague and Harrison [17] are approximately 40% below the sum of the two subshell cross sections at the peak of the data. The agreement between experiment and the configuration-average distorted-wave calculations for W^+ is typical for neutral and few-times ionized complex atoms. The Lotz results are found using Eq. (3) with $q=1$ for the $6s$ subshell and $q=4$ for the $5d$ subshell. We again note that no shape resonances appear in the subshell ionization cross sections for W^+.

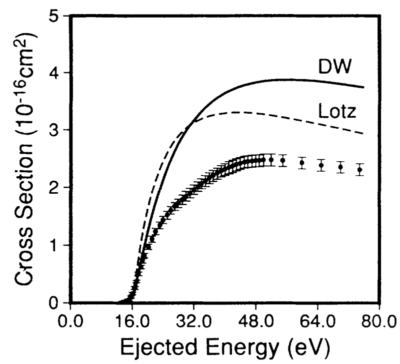

FIG. 3. Total cross section for the electron-impact ionization of W^+. Solid curve is the sum of distorted-wave results for the $6s$ and $5d$ subshells; dashed curve is from the Lotz formula; experimental measurements are from Montague and Harrison (Ref. [17]).

In conclusion, the configuration-average distorted-wave calculations for the various subshell ionization cross sections of neutral W have uncovered a giant shape resonance. Although the present calculations need to be extended to include intermediate-coupling and configuration-interaction effects in order to make more precise the strength of the shape resonance, a strong feature should be observable in the total-ionization cross section. We further suggest that the best place to search for both shape and compound resonance structures in electron ionization of atoms and their ions is in the differential cross section with ejected energy.

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