§7. Ionization of Mo, Mo$^+$, W, and W$^+$ by Electron Impact

Kim, Y.K. (NIST, USA),
Zou, S.Y. (Grad. Univ.)

The valence shells of Mo ($4d^5 5s$, $4d^4 5s^2$), Mo$^+$ ($4d^5$, $4d^4 5s$), W ($5d^4 6s^2$) and W$^+$ ($5d^4 6s$, $5d^3 6s^2$) have nearly half-filled d shells, resulting in a large number of low-lying metastable levels that share the same electronic configurations as the ground states. This complex valence structure poses a daunting challenge for collision theories to calculate cross sections for ionization by electron impact.

There has been no report of experimental ionization cross sections for Mo and W probably because of their low vapor pressure, though theoretical ionization cross sections have been reported for Mo by Badnell et al. [1] and for W by Pindzola and Griffin [2]. On the other hand, experimental data for the ionization of Mo$^+$ [3, 4] and W$^+$ [5, 6] are available. Pindzola and Griffin [2] also reported theoretical ionization cross section for W$^+$, but their peak cross section is ~60% higher than the two sets of experimental data, which agree with each other.

To address the issue of ionization, the binary-encounter-Bethe (BEB) model [8] is used to calculate the direct ionization cross sections, and the scaled Born cross sections [9, 10] is used to determine the contributions from excitation-autoionization. In our theory we have included possibilities that (a) some target atoms used in an experiment were in metastable states close to the ground state, (b) autoionization via the $4p/4d \to 4d/4f$ excitations in Mo/Mo$^+$ and $5p/5d \to 5d/5f$ excitations in W/W$^+$ may be substantial, and (c) ions produced in experiments may be in excited, low-lying metastables. Due to the huge number of metastable states, it is impractical to track all fine-structure levels; only an "average J" used in this calculation. The preliminary results of this calculation are shown in Figs. 1 and 2 together with the available experimental data [3, 4, 5, 6] and other theoretical calculations.

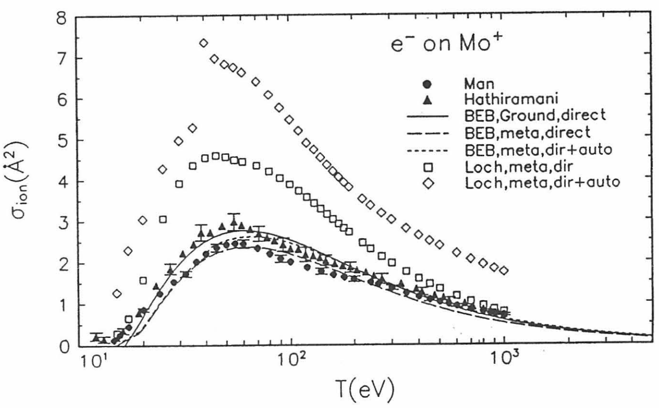

Fig 1. Ionization cross sections for Mo$^+ \to$Mo^{2+}

The BEB cross sections for Mo$^+$ is in good agreement with the data by Harthiramani et al. [4] except near the threshold. In Mo$^+$, experiments indicate strong autoionization near T=15 eV, and the shape of the peak reported in [4] suggests another group of autoionization near the peak. Our theory did not add much to the cross section of Mo$^+$ near T=15 eV from the hunderds of the $4d \to 4f$ excitations examined. The threshold for hundreds of the $4p \to 4d$ excitations in Mo$^+$ are near T=40 eV, thus contributing to the unusual shape of the peak. The BEB cross section for W$^+$ is in better agreement with the data by Montague et al. [5] at low incident energies than the data by Stenke et al. [6]. Comparisons to experiments for Mo$^+$ and W$^+$ exhibit overall agreement between the BEB model and experiments, indicating that excitation-autoionization is insignificant near the cross section peak.

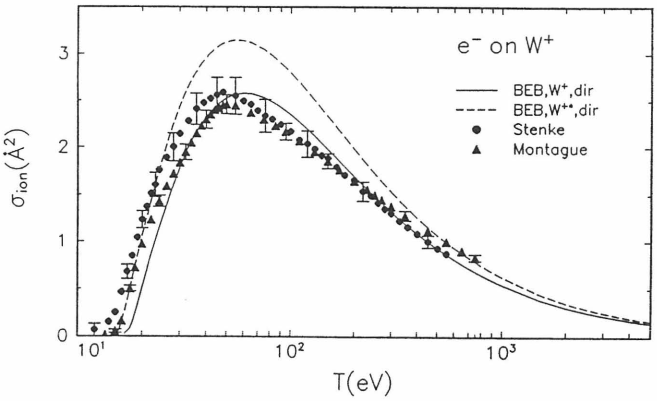

Fig 2. Ionization cross sections for W$^+ \to$W^{2+}

To clarify the ionization mechanism, we have more work to do. Calculate auoionization contributions to the ionization of W$^+$ using diploe/spin allowed excitation and compare to available experiments.

The good agreement of present cross sections for the ions indirectly support the reliability of our cross sections for Mo and W.

References

1. N. R. Badnell, T. W. Gorczyca, M. S. Pindzola, and H. P. Summers, J. Phys. B **29**, 3683 (1996).
2. M. S. Pindzola and D. C. Griffin, Phys. Rev. A **46**, 2486 (1992).
3. K. F. Man, A. C. H. Smith, and M. F. A. Harrison, J. Phys. B **20**, 1351 (1987).
4. D. Harthiramani, K. Aichele, G. Hofmann, M. Steidl, M. Stenke, R. Völpel, and E. Salzborn, Phys. Rev. A **54**, 587 (1996).
5. R. G. Montague and M. F. A. Harrison, J. Phys. B **17**, 2707 (1984).
6. M. Stenke, K. Aichele, D. Harthiramani, G. Hofmann, M. Steidl, R. Völpel, and E. Salzborn, J. Phys. B **28**, 2711 (1995).
7. S. Loch, private communication (2002), for Mo, Mo$^+$.
8. Y.-K. Kim and M. E. Rudd, Phys. Rev. A **50**, 3954 (1994).
9. Y.-K. Kim, Phys. Rev. A **64**, 032713 (2001).
10. Y.-K. Kim, Phys. Rev. A **65**, 0222705 (2002). .