

CLOSE-COUPPLING R-MATRIX APPROACH TO SIMULATING ION-ATOM COLLISIONS FOR ACCELERATOR APPLICATIONS*

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Abstract

We have used an R-matrix close coupling algorithm to calculate capture, ionization and excitation cross sections for 0.5 to 8.0 MeV K⁺ incident on argon and neon. These energies, ions and gasses are relevant to the High Current Experiment (HCX) at Lawrence Berkeley National Laboratory, where impact ionization of background gasses is a main source of contaminant electrons. The R-matrix close coupling algorithm is a semi-classical algorithm that uses quantum mechanics to describe the particle interactions and classical mechanics to describe the nuclei trajectories. We find for argon, ionization and capture cross sections are roughly equal and on the order of a few 10^{-17} cm². For neon, we find the cross section for ionization is a few 10^{-16} cm², while the cross section for capture is a few 10^{-17} cm².

MOTIVATION AND APPROACH

We use the R-matrix close coupling algorithm developed by Lee *et. al.* [1,2]. This two-center approach approximates the projectile and target as radial pseudo-potentials, typically with a four-parameter fit to describe the potential. One chooses the parameters by how well the pseudo-potential reproduces known ionization values.

$$V(r) = -\frac{1}{r}(z_0 + (z_1 + z_2 r)e^{-z_3 r}) \quad (1)$$

For our simulations, we use $Z_0=-1$ for all centers. For neon, we used $Z_1=9$, $Z_2=17.2$, and $Z_3=3.0$. For argon, we used $Z_1=17$, $Z_2=-3.0$, and $Z_3=2.15$. For potassium, we used $Z_1=18$, $Z_2=-2.2$, and $Z_3=2.04$.

One then solves the time-dependent Schrödinger equation for the one active electron (initially on the target), assuming the two centers follow classical trajectories. To account for the presence of two electrons in the outer shell of argon and neon, we multiply our results by a factor of two. The authors of ref. [3] present a more accurate treatment of the case of two active electrons, but we have not implemented this yet.

From the energy of the final state, we can determine three separate events. If the electron, which started in a bound state on the target, transitions to a bound state of the projectile, capture has occurred. If the electron transitioned to a different bound state on the target, excitation has occurred. Finally, if the electron finishes in an unbound state on the target, ionization has occurred.

Figure 1 shows the numerical results for the cross section for excitation, ionization, and capture calculated in this way for K⁺ on argon and neon for a range of energies relevant to the HCX. We find for argon, ionization and capture cross sections are roughly equal and on the order of a few 10^{-17} cm². For neon, we find the cross section for ionization is a few 10^{-16} cm², while the cross section for capture is a few 10^{-17} cm².

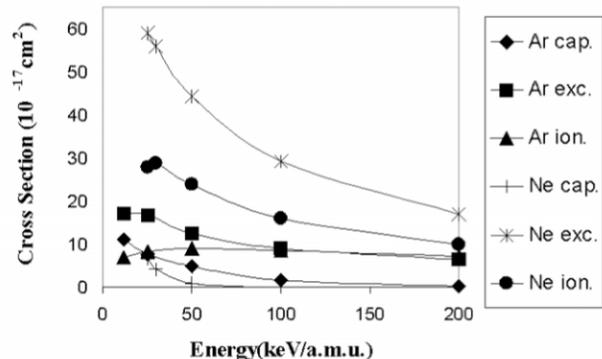


Figure 1: Comparison of excitation, ionization, and capture cross sections for neon and argon targets as a function of energy for a singly-ionized potassium projectile.

REFERENCES

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