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MULTIPLE IONIZATION CROSS SECTIONS BY ION IMPACT ON Ne-like MOLECULES



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Abstract

Single and Multiple Ionization Cross Sections (MICS) by ion impact on Ne and Ne-like molecules are calculated in the framework of the Independent Electron Model (IEM) and taken into account post-collisional effects like Auger and Coster-Kronig processes. The single particle probabilities in the MICS, are represented by decreasing exponential functions, called the **Exponential Model (EM)**. The net ionization cross sections by atomic o molecular orbital required as input by the EM, are calculated using the CDW-EIS approximation. The MICS calculated with the EM probabilities are in very good agreement with experimental data and present better agreement than other more complex theoretical models

Ne, CH_4 , NH_3 and H_2O

Processes for target electron loss:

- Single and multiple Ionization
- Electron capture



- Auger-like ionization processes
- Very important at high projectile energy!

Multiple ionization Cross Sections





Theoretical Model

Independent Electron Model

The collision is seen as a product of independent interactions between the projectile and the target electrons. Electron correlation is not considered

Q- fold Ionization Cross Section



Galassi M E, Rivarola R D, and Fainstein P D 2007 Phys. Rev. A 75 052708



Exponential Model (EM): single particle probability for ionization

$$p_i(b) = p_{i0}e^{-b/r(i)}$$
$$r(i) = \frac{n_i^2}{\sqrt{-2n_i^2\varepsilon_i}}$$

The parameter p_{i0} is determined to reproduce CDW-EIS total cross sections for single-electron emission per electron for each orbital

Carlson et al. Phys. Rev. 151 (1966) 151-47

Ne

NH₃

Atomic Orbital	Populations	Binding energy (eV)
1s	2	-891,4
2s	2	-52,5
2р	6	-23,13

CH₄

Molecular Orbital	Populations	Binding energy (eV)
C1s (2)	2.00 C1s	-290.7
2.5 (2)		00.0
2a ₁ (2)	1.133 C2S + 0.867 H1S	-22.9
1 <i>t</i> ₂ (6)	3.399 C2p + 2.601 H1s	-12.6

Conclusions

 \succ Multiple Ionization Cross Sections of Ne, H2O, NH3 and CH₄ by ion impact were obtained applying the Independent Electron Model and taken into account post-collisional effects.

>The results obtained using EM single particle probabilities + post-collisional effects are in very good agreement with experimental data.

>Post-collisional effects dominates the Double Ionization Cross Sections for energies higher than 1 MeV for proton impact, but it depends on the ionization degree.

 \gg We will continue investigating the applicability of the EM-MICS model to describe the fragmentation channels of Ne-like molecular targets.

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