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Improvement of the ETACHA Code towards low velocities and many-electron ions

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Synopsis Knowledge of the detailed evolution of the whole charge state distribution of projectile ions colliding with targets is required in several fields of research such as material science, atomic, plasma and nuclear physics, in particular in regards of the several foreseen large scale facilities. Starting from the previous ETACHA model [1], we present extension of its validity domain towards lower velocities and larger distortions. Moreover, the system of rate equations is now able to take into account ions with up to 60 electrons.

Ab initio calculations of charge state distributions of fast ions at the exit of solid targets are useful in many circumstances, as in the context of energy loss in matter and for the design, or analysis, of atomic, plasma or nuclear physics experiments. Several empirical or semi empirical laws can be used to predict the mean charge state at equilibrium [2], however, in many cases, the detailed evolution of the whole charge state distribution as a function of the solid target thickness or even the evolution of the $n\ell$ substate populations are needed. The initial version of the ETACHA code [1] intended to calculate charge state distributions of fast few-electron ions with at most 28 electrons. It was therefore based on calculations of cross sections for monoelectronic atomic collision processes in the independent electron approximation and at high velocities. However, in the present days, many experiments take place in the non-perturbative regime, where previously used Born1 type calculations break down. Moreover, more states have to be included.

Several improvements have been made. More refined calculations are performed for ionization and excitation, namely, the Continuum Distorted Wave-Eikonal Initial State and Symmetric Eikonal approaches respectively. In parallel, studying carefully the evolution of cross sections of projectile electron-gain, -loss and -excitation versus the principal quantum number n, we also extend the applicability of the code up to dressed ions with (in principle) 60 electrons, i.e. with full *n*=4 shell.

Comparison with experiments for systems such as 28.9 MeV/u Pb⁵⁶⁺ ions in carbon (see Fig.1) shows

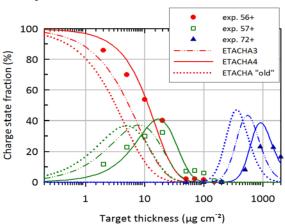


Figure 1. Evolution of selected charge states for 28.9 Mev u⁻¹ Pb⁵⁶⁺ with carbon target thickness. Symbols: experiment [2]; dotted lines: ETACHA "old" [1]; dashed-double-dotted lines: ETACHA3 (up to n=3); full lines: ETACHA4 (up to *n*=4).

very good agreement with the new fully ab initio calculations of the ETACHA code. It demonstrates that even for a projectile initially dressed with 26 electrons, i.e. Pb⁵⁶⁺, it is mandatory to properly take into account n=4, because here the excitation from n=3 to n=4 is as large as the ionization of n=3. This new version of the ETACHA code provides also accurate predictions for other systems like 0.05 -0.5 MeV/u C ions in aluminum which is of interest in warm dense plasma experiments [3].

References

[1] Rozet J P, Stéphan C, and Vernhet D 1996 Nucl. Instrum. Meth. B 107 67-70 [2] Leon A et al. 1998 Atomic Data and Nuclear Data Tables 69, 217-238 (and references therein) [3] Gauthier M et al. 2013 Phys. Rev. Lett. 110, 13500

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