First-Principles–Simulation of Charge State and Stopping Power of Swift Heavy Ions in Solids and Plasmas ◊

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Up today there exists no closed theory for calculating both charge exchange and energy loss of heavy ions in solids. We have thus developed an approximation to this longstanding problem in terms of simulating a classical many-body system interacting exclusively via *pure* Coulomb's Law, thus a treatment from first-principles, where charge exchange and energy loss are calculated on *equal* footing [1].

All previous stopping theories have as a matter of fact (at least) two open parameters, namely the projectile's charge state as well as its excitation state. While stopping is in its most simple form a two-body process, charge exchange involves at least three particles for momentum and energy conservation. As it turns out in our calculations the most typical case is *multiple* electron capture and loss with *simultaneous* many-target atom interactions.
So far a comparable intensive investigation of the projectile charge state seems indeed lacking. Instead, "effective" charges have been introduced which, basically spoken, merely serve as fitting parameters, even if the often used Thomas-Fermi scaling laws pretends a deeper understanding.

A treatment of both ion charge and stopping power on *equal* footing immediately rules out any quantum theoretical approach, since especially charge transfer processes between multi-electron atoms and ions is an unsolvable task up to now [2]. We have therefore extended the so-called "n-body Classical Trajectory Monte Carlo" (nCTMC) [3] procedure to be applicable for the interactions of swift ions in *solids* where the ion interacts *simultaneously* with N target atoms each carrying n electrons, thus calling our code nN-CTMC [4] in contrast to nCTMC where only *single* ion-atom collisions are treated.

In this code the temporal evolution of a classical many-body system is calculated, based upon Newtonian mechanics. This system consists of target nuclei and orbiting bound electrons, as well as the projectile nucleus and bound projectile electrons. All particles interact with each other, except bound target electrons among themselves. The initial conditions, such as binding energies and radii, are taken from single-configuration Hartree-Fock calculations. The simulation generates large statistical ensembles selecting the initial condition of each run by a random number generator among all possible conditions and then delivers mean values, e.g. mean stopping powers averaged over many independent runs. The result for 1 MeV/u Ni ions in a carbon foil is given in Fig. 1. One can clearly see that all ions tend towards an equilibrium charge state independent from the initial charge. The higher the initial charge state the higher is the corresponding stopping power and the equilibrium stopping power is again independent from the initial charge state. Not only the equilibrium charge state, but also its total distribution, as well as the equilibrium stopping power and even the depth for reaching equilibrium is in close agreement to experimental data. This underlines the capability of our simulation, also supporting to extend it to parameters which are experimentally not accessible, such as excitation states and non-equilibrium stopping powers at the surface of the target.

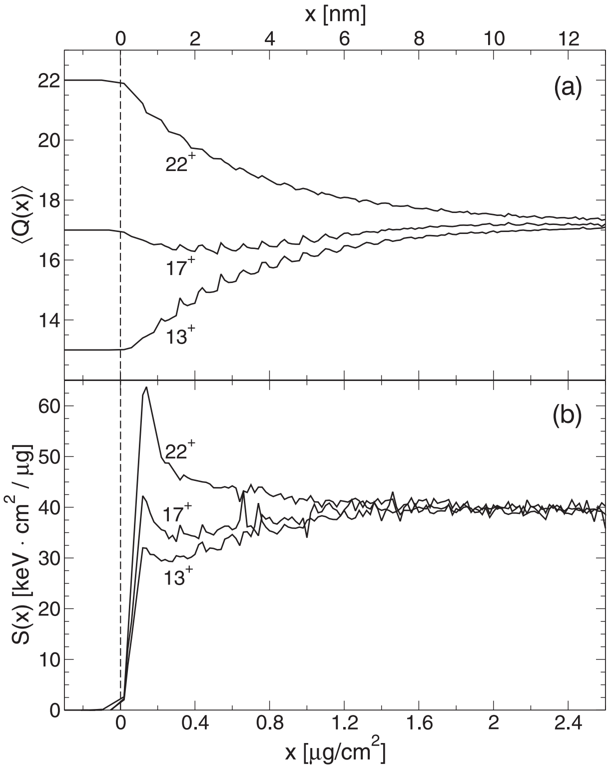

Fig. 1: Mean charge states (a) and corresponding stopping power (b) of 1 MeV/u Ni ions vs. penetration depth x in a 14nm thin carbon foil for three different initial charge states $Q_{in} = 22, 17, 13$.

In our group a new version of nN-CTMC is devoted to calculate the stopping power in dense plasmas. In a first approach a fully ionized plasma is simulated, thus all electrons are free and homogenously distributed within the simulation box. It is well-known that stopping is stronger in plasma than in the corresponding cold matter, for which two reasons are discussed. One is the higher charge states, as ions cannot capture free electrons, and secondly a larger cut-off in the impact parameter dependence of stopping power. It is the aim of our simulation to reproduce measurements performed with 3.9 MeV/u Ar ions at GSI. Such a first-principles–simulation can deliver microscopic views on stopping in plasmas, including the degrees to which the two arguments above contribute to the enhanced stopping.

References

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