Electronic Stopping of Heavy Ions in the Kaneko Model

R. Mathar and M. Posselt

Two quantities determine the electronic stopping of heavy ions from the point of view of effective charge theory: (i) the radial charge distribution of the electrons that are bound to the ion, or rather its wave number representation. The ionization fraction as a function of the ion velocity and atomic number is the key entry. (ii) The dielectric function of the target as a function of wave number and frequency. Together they define the polarization charges that are created by the moving ion, and finally the force (stopping power) that these charges exert on the ion. The name 'effective charge' points out that, under the restriction of a linear susceptibility of the target, the stopping cross section of partially stripped ions is not simply the squared ion atomic number times the proton stopping cross section at the same velocity, but effectively smaller.
The familiar theory based on the work of Brandt et al. [1, 2] deals with the target model of a homogeneous free electron gas (FEG). The essential contribution of the inner target shells to the target polarization is therefore missing, and experimental proton data, which evidently contain this piece of information, are scaled to obtain reliable results.
A more fundamental theory has been set up by Kaneko [3]. It delivers formulas for the susceptibilities of individual shells of bound electrons of target atoms. They may be roughly interpreted as a generalization of the calculation of the susceptibility of a FEG [4] to lowest order, but the momentum distribution of the wave packets of bound electrons is approximated by a Gaussian instead of the 'Fermi ice block.' The total stopping power is finally written down as a sum of target subshell contributions. Theories of this kind can compute heavy ion stopping powers without recourse to proton stopping powers. Nevertheless, the model has almost exclusively been applied to light ion stopping. Searching for improvements of the theory and its application to heavy ion stopping we discussed four aspects [5]:
(1) **Energy gaps of target shells.** We included a correction to the susceptibilities of shells

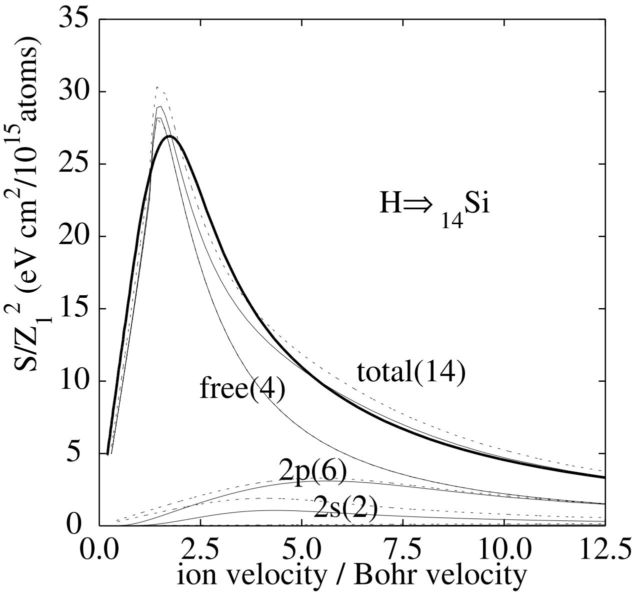

Figure 1: Total and per shell proton stopping cross sections in $_{14}$Si. Dotted lines: Original Kaneko theory. Bold: ZBL [2]. Thin solid lines: theory with energy cuts of the Si $1s^2$, $2s^2$ and $2p^6$ shell. Occupation numbers of the shells are given in parentheses.

of bound electrons to take into account that an electromagnetic field must at least transfer the energy of the individual excitation gap of the bound target electron [6] in order to create a (real) electron-hole pair. Polarizations and stopping powers are diminished by this kind of low-energy cut of the imaginary part of the susceptibilities, and the stopping powers of the subshells concerned no longer rise linear at low ion velocities. Looking at the stopping powers of protons, the general 5 – 10 % overestimation of their high-velocity stopping is removed (fig. 1). Because energy gaps change only features of the target model, protons are chosen here to remove the uncertainty on the projectile charge distribution from the theory. The action on heavy ion results is equivalent (cf. fig. 2).

(2) **Dead sphere of polarization.** The Kaneko theory more and more overestimates heavy ion stopping powers at their maximum, when the ion atomic number increases. We discovered that this corresponds to the feature of the familiar formulas to allow a target polarization without restriction on space. In a more realistic calculation, the electrons bound to the ion occupy some domain. We call it a 'dead sphere', since the excitation of a target polarization of either sign is suppressed there: target electrons cannot penetrate into this sphere, because the electron density inside is already fixed by the atomic theory; target electrons are not scattered from inside the sphere, because there are hardly any inside. This model to remove the polarization at the close neighbourhood of the ion nucleus lets the ion no longer 'skim over' but 'plough through' the target electrons. It is strongly supported by the observation that fits of the radii of these dead spheres are roughly equal to the radii of the outer shells of partially stripped heavy ions (fig. 2).

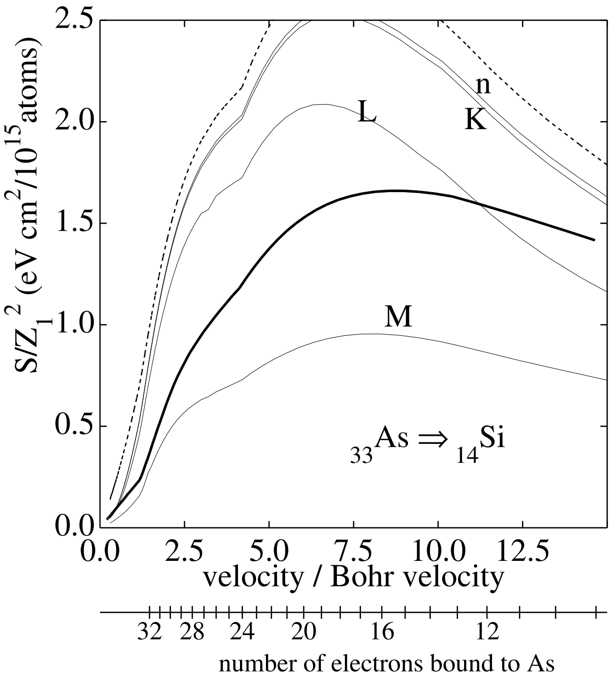

Figure 2: $_{33}$As electronic stopping in $_{14}$Si. Bold line: ZBL [2]. Dotted: original Kaneko theory with ZBL ion parameters. Thin solids: Kaneko theory with energy cuts of Si shells. Line 'n': no dead sphere. Lines 'K', 'L' and 'M': dead sphere radius set to the corresponding ion shell radius. Z_1 is the ion atomic number. Fig. 3 presents an example, where the dead sphere radius is dynamically shrunk with the ion size.

In the framework of effective charge theory, which defines the effective charge from the statistics of close and distant collisions between the ion and the target electrons, our rejection of some contribution to the 'close' channel inevitably reduces the effective charge. The calculation defines some effective new ion form function and is therefore not tied up with a special target model.

Light ions — at least up to $_5$B — are best fitted by the original model without dead sphere, even if some electrons are bound. Obviously, the expulsion of target electrons from the ion core needs a minimum interior electronic density to become effective.

(3) **Susceptibilities of target p and d subshells.** Height and location of the stopping maximum of *light* ions are dominated by the contribution of the free target electrons, the maximum of

heavy ions more by the next inner, usually 2p and 3d, shells (fig. 1 vs. fig. 3, for example). We therefore checked another prospective reason for a new treatment of p and d subshells to explain the different success of the previous light and heavy ion computations.

The Kaneko theory assumes a Gaussian momentum distribution of the electron ground state of target shells as a starting point. This kind of wave packets was derived from thermodynamics without reference to an atomic theory. If we look at Fourier representations of free-atom Roothaan–Hartree–Fock electronic densities [6], and average over the directions of the momentum, this ansatz is confirmed for s shells, but a multiplication of the Gaussian with powers of the momentum is superior for shells with non-zero angular momentum quantum number. We recalculated the susceptibilities of these generalized ground states within the random phase approximation, but the change of the stopping powers turned out to be small (fig. 3).

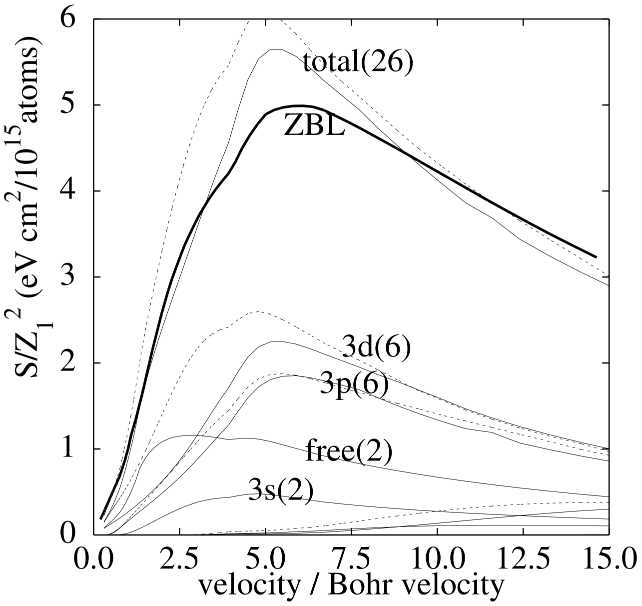

Figure 3: Total and per shell $_{15}$P stopping cross sections in $_{26}$Fe. Bold line: ZBL [2]. Dotted: Kaneko theory with the plain Gaussian form of the electron wave packets in the ground state of Fe shells. Thin solid lines: Theory with the modified susceptibilities of the $2p^6$, $3p^6$ and $3d^6$ Fe shells. All non-ZBL results used a dead sphere radius of 1.1 times the ZBL ion size parameter, and cut energies for Fe shells.

The representation of d bands of solid transition metal targets by free-atom d orbitals, however, is questionable. Our (with respect to the angular momentum quantum number of the target shell) non-degenerated new formulas are therefore thought not advisable, and a better tuning is desirable in these cases.

(4) **Mutual (anti)screening and interaction of target shells.** The Kaneko theory sums up the polarization charges of all target shells independently. One artifact of this procedure is, for example, the overcompensation of the ion charge by the total polarization charge. We have tested an improved version of the theory, where the target polarization is not solely invoked by the field of the passing ion, but by the total field of the ion plus the remaining shells. It means building the target dielectric function by one plus the sum of all shell susceptibilities, and is equivalent to switching on a (Hartree) interaction between the polarization charges of different target shells. The overall change of stopping powers is modest, except for the extinction of the contribution of free-electron plasmons in transition metals — the concurrence and overlay of their excitation spectra with the damped excitations of the 3d shell makes them effectively decay into 3d single-particle excitations.

The Kaneko theory provides a computation of electronic stopping powers in random targets which is parameter-free with respect to the target. Our most essential contribution to the dielectric theory was the installation of a polarization-free sphere around the nuclei of partially stripped ions to explain the systematic overestimation of the stopping power of heavy ions as a function of atomic number.

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