Improved accuracy of the code ATIMA for energy loss of heavy ions in matter

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The precise knowledge of the energy loss of heavy ions penetrating through layers of matter is essential for experiments, heavy ion therapy, separation of projectile fragments and many more accelerator applications. The program ATIMA (ATomic Interaction with MAtter) predicts the energy loss, energy-loss straggling and angular scattering of ions penetrating matter. Its predictions compared to data measured at the fragment separator FRS have demonstrated that an accuracy of ~1% in the stopping force (dE/dx) can be achieved. This has been accomplished for bare ions by using the LS-theory [1], whereas the pure Bethe theory deviates up to 10% [2] and by up to a factor of two in energy-loss straggling for high projectile atomic number (Z_1) ions at 1 GeV/u [3]. However, for ions with a few or many electrons the simple charge formula of Pierce and Blann [4] used in the ATIMA up to version 1.3 is not accurate [5], because it is not dependent on the target material. The experimental data also show that with an improved projectile mean charge description a good agreement can be achieved for high Z_1 ions (Au-U) down to 100 MeV/u where the K and L shells are partially filled.

Compared to the many mean charge formulas, theory-based analytical cross sections work best at sufficiently high velocity, as theory distinguishes correctly between the various electron capture and ionization processes. Yet for lower velocities the involved perturbation theory shows significant deviations. Based on the large amount of measured data with the FRS, a simple correction to the results from the GLOBAL program [6] with only three parameters was derived. The calculated mean charge depends on the velocity, the projectile (Z_1) and the target material (Z_2). This new description implemented in ATIMA, works for the entire range of projectile and target combinations down to 40 MeV/u.
Figure 1 shows the mean charge state prediction of uranium projectiles compared to our experimental data. The predicted mean charge varies considerably with Z_2, from <q>=86.2 in Be down to <q>=79.6 in Pb at 30 MeV/u. For even lower energies down to 10 MeV/u a pure fit formula [7] is used. For smoothening in the transition region a weighted average is used.

Unlike most other programs, in ATIMA we use the mean charge as it can be observed directly in experiments, whereas often an effective charge is used in stopping-power predictions to adjust for many effects. All other contributions to dE/dx are described by separate formulas such as the Barkas effect, shell corrections, and the Fermi-density effect [8]. With this approach we can gain a deeper understanding and improve the theoretical descriptions.

The accuracy of our new description has been tested with experimental data of projectiles with many electrons and different materials. The experimental data have been collected with the FRS in the last decades. This is an independent test as none of these measured data was used as a parameter in ATIMA 1.4 except for the mentioned mean charge. The data include U, Bi, Pb, Au, Xe, Kr, Ni projectiles on mainly solid targets ranging from Z_2=4 to 82 with energies from 1000 MeV/u down to 45 MeV/u.

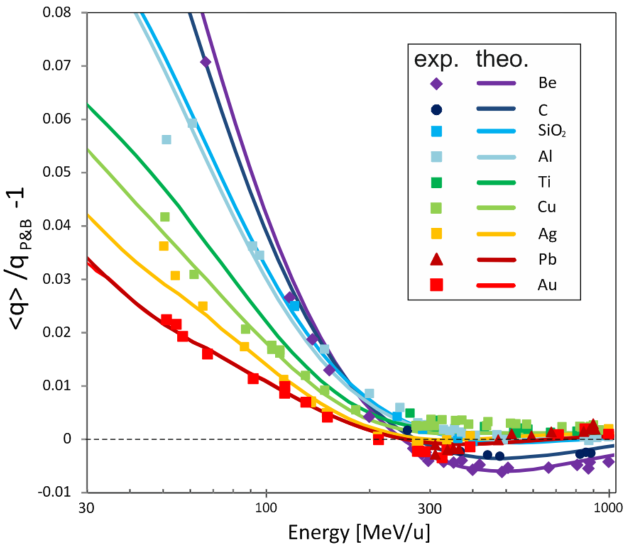

Figure 1: New predictions for the mean charge states of uranium ions after penetration of different target materials as function of energy are compared with experimental data. The comparison is normalized to the simple mean charge formula [4] used in the previous ATIMA versions.

Figure 2 shows a comparison of measured and predicted stopping forces in the energy range with the biggest differences to the previous ATIMA. The improvement is clearly demonstrated. In a limited energy range other programs, based on fits to measured data [9, 10], are better than the previous ATIMA version, but they fail for higher energies due to the simple effective charge approach and missing fully relativistic theory. At high energies for bare ions the results of ATIMA are accurate and remain unchanged.

The comparison of ATIMA 1.4 with experimental data includes all the available measured dE/dx values above 30 MeV/u. Table 1 shows the average standard deviations to theory from five experiments with the FRS. For the listed average relative standard deviations, the differences were weighted with the experimental errors. Of course the accuracy of the comparison is limited by the experimental errors.

For the data of ref. [11] up to 1 GeV/u with mainly bare ions ATIMA 1.4 naturally yields only a small improvement, but theories based only on perturbation theory show large deviations. The data of ref. [12] for Au-Bi ions in the range of 110 to 880 MeV/u with projectiles carrying a few electrons can be described better with ATIMA1.4. The same holds for the data of ref. [13] for Xe ions in the energy range of 60 to 290 MeV/u. The new yet unpublished Uranium data down to 80 MeV/u with many electrons require ATIMA1.4. In this case the remaining deviations are only as small as the experiment errors themselves, while ATIMA1.3 - and other formulas even more - deviate significantly. At even lower energies (ref. [14]) the charge prediction and also the Barkas and shell corrections become less accurate, which explains the larger remaining deviation to ATIMA 1.4. Here the simple charge formula of ATIMA1.3 is not useful anymore as could already be seen in the comparison of Figure 1. Still ATIMA 1.4 is slightly better or is as good as the fit formulas.

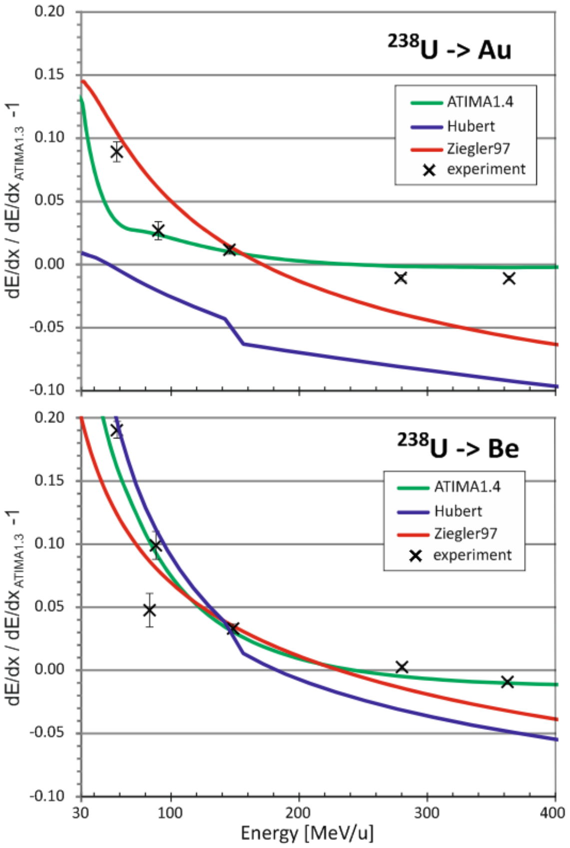

Figure 2: Comparison of new experimental dE/dx values of uranium ions in Au and Be targets to different formulas.

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Table 1: Comparison of experimental data for different projectiles (Z_1) and number of data points (N) with different theories: ATIMA1.3 ATIMA 1.4, Hubert [9], and Ziegler97 [10]. Listed are the average relative experimental errors and the average deviations of the theory from experimental data.

			[%]	[%]	[%]	[%]	[%]
Ref.	Z_1	N	exp.	A1.3	A1.4	Hub.	Z97
[10]	8-92	31	1.9	0.88	0.84	8.6	6.7
[11]	79-83	41	1.1	1.8	1.3	8.1	6.1
[12]	54	21	0.84	2.6	1.5	3.4	2.7
[13]	92	21	2.2	10.0	3.6	4.6	3.3
new	92	23	0.78	1.5	0.78	5.0	1.8

In the energy region much below 100 MeV/u the gas-solid difference in stopping powers of heavy ions makes the description more difficult. The gas-solid difference has been discovered at GSI about 40 years ago and has been confirmed in many experiments [15]. New experiments (approved proposal S469) are planned in different gaseous or solid targets.

Presently, below 10 - 30 MeV/u the region where direct theory becomes unreliable fit formulas with an effective charge as a variant of Ziegler's code [10] are applied in ATIMA and in addition a calculation for the contribution by elastic atomic collisions.

Since ATIMA version 1.3 the calculation includes projectiles up to Z_1=120 and targets up to Z_2=99 based on extrapolations. On the higher energy side ATIMA 1.4 calculates up to 450 GeV/u and also includes the then important nuclear size effect of the projectile [1, 8].
Integration of ATIMA into other programs such as MOCADI [16], PHITS [17], GEANT4, or ion optical codes has been done or is in progress. For an easy application, we provide a program as an interface to pre-calculated tables, as well as an online calculator [18].

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Experiment beamline: FRS
Experiment collaboration: NUSTAR-SuperFRS-Experiments
Experiment proposal: S469
Accelerator infrastructure: SIS18 / FRS / Super-FRS
PSP codes:
Grants: SATNURSE EU project number 654002
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