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Simulation of ion beam scattering in a gas stripper

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ABSTRACT

Ion beam scattering in the gas stripper of an accelerator mass spectrometer (AMS) enlarges the beam phase space and broadens its energy distribution. As the size of the injected beam depends on the acceleration voltage through phase space compression, the stripper becomes a limiting factor of the overall system transmission especially for low energy AMS system in the sub MV region. The spatial beam broadening and collisions with the accelerator tube walls are a possible source for machine background and energy loss fluctuations influence the mass resolution and thus isotope separation. To investigate the physical processes responsible for these effects, a computer simulation approach was chosen. Monte Carlo simulation methods are applied to simulate elastic two body scattering processes in screened Coulomb potentials in a (gas) stripper and formulas are derived to correctly determine random collision parameters and free path lengths for arbitrary (and non-homogeneous) gas densities. A simple parametric form for the underlying scattering cross sections is discussed which features important scaling behaviors. An implementation of the simulation was able to correctly model the data gained with the TANDY AMS system at ETH Zurich. The experiment covered transmission measurements of uranium ions in helium and beam profile measurements after the ion beam passed through the He-stripper. Beam profiles measured up to very high stripper densities could be understood in full system simulations including the relevant ion optics. The presented model therefore simulates the fundamental physics of the interaction between an ion beam and a gas stripper reliably. It provides a powerful and flexible tool for optimizing existing AMS stripper geometries and for designing new, state of the art low energy AMS systems.

1. Introduction

The interaction of particles with matter has been studied for decades. It was found that particles traveling through a target lose energy and are deflected from their initial direction. An explanation was given by Rutherford [1] who has shown that elastic collisions of atomic nuclei are responsible for large scattering angles. For heavy projectiles and low energies, this is the dominant process for energy loss of ions in matter and is known as nuclear stopping. Inelastic collisions comprise ionization of ions or target atoms and electron capturing. This is a crucial process for accelerator mass spectrometry (AMS) to remove molecular mass interferences from the analysis by selecting high ionizations states of a particle beam. Molecules become instable if too many electrons are stripped off them, the interfering molecules thus dissociate [2], which effectively removes them from the ion beam after filtering for mass. In AMS, this is done in an (electron) stripper, a target of solid or gaseous form. By using this technique though, a fraction of the beam is lost through selection of the respective charge state as multiple charge states are produced through stripping. The only way to minimize these losses is the choice of the right energy range, as the population of charge states depends on the ion velocity for a given stripper medium. With advances of AMS systems towards low energy [3] and heavy ion [4] applications, the weaker phase space compression of the ion beam and increased angular straggling leads to additional ion losses in the stripper. As all lost ions are not available anymore for detection, the measurement precision is decreased through lower counting statistics. An example is the comparison of a well optimized radiocarbon AMS system running at 200 kV [5] with a system running at just 45 kV [3] showing an increase in scattering losses by a factor of two to three. Furthermore, scattering of ions with the walls of the stripper tube or their interaction with residual gas can be a possible source for detection background since these particles may travel on skewed trajectories through the system and might end up in the final detector [4]. To build compact systems operating at low ion energies it is hence of crucial importance to optimize the stripper to maximize transmission and minimize creation of detection background.

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The ion optical transport of ions through an AMS system is well understood and is often already modeled through simulation programs like GICOSY [6] and analyzed in detail [7]. The influence of the stripper medium on the ion beam has mostly been estimated with analytical solutions of approximations of multiple scattering theory [8]. Another approach to tackle this is the use of simulation codes like TRIM [9,10].

The fundamental processes of nuclear stopping may be broken down to a binary elastic collision problem which is well described in today's physics courses. The distribution of scattering angles was described by Rutherford [1] and extended to full, electron screened atoms [11,12] in form of simple formulas by Winterbon [13]. This encouraged us to develop a new tool to simulate single scattering events of ions in an AMS gas stripper and investigate their influence on the entire ion beam. With AMS in mind, it is simple to connect the tool to further simulations like ion optics and to include real gas density distributions. In the first part of the paper, the fundamental principles of scattering probabilities in a screened Coulomb potential and two body scattering kinematics will be described. It will be discussed how they can be modeled in a computer program. In a second part we will present how this can be used to model ion beam transmissions through the system and explain the form of beam profiles, which are observed after stripping with the comparison to measurements at one of our AMS systems.

2. Methods

2.1. Scattering simulation algorithm

2.1.1. Overview

To describe the trajectory of an ion passing through a gas (Fig. 1), the scattering algorithm presented in this paper deals with the process responsible for angular straggling in matter: elastic collisions of the ion with single gas atoms in a screened Coulomb potential. This section gives a brief overview over the full simulation, the individual steps of the whole process are explained in more detail in the sections below.

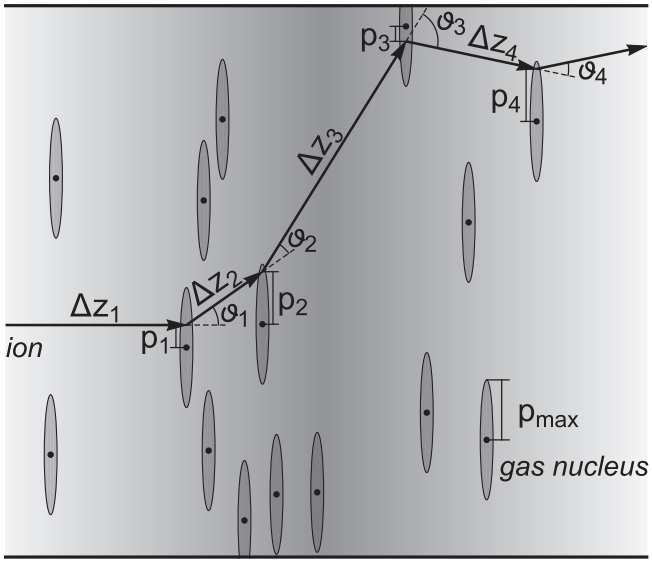

Fig. 1. The model of a gas stripper with inhomogeneous density (highest in the center). Single targets in form of gas nuclei are indicated with their geometrical interaction cross sections (radius p_{max}) as seen from an incident ion from the left side. The ion travels freely with path lengths Δz_i until it scatters off a gas atom at an impact parameter p_i, leading to a deflection with scattering angle ϑ_i. For simplicity, the process is considered in a longitudinal section of the stripper tube only.

The algorithm may be divided into three main tasks. They are repeated in an iterative manner to track the ions path through the medium until it either leaves the medium or hits the stripper tube wall and is considered lost. Between single elastic collisions with the gas nuclei of the medium, the ion travels freely until the transverse distance p_i to a nucleus, the so called impact parameter, falls below a certain threshold p_{max}. The first task deals with the determination of this free path length Δz_i based on the gas density and event cross section and thus dictates the next point of elastic collision. The outcome of this single interaction depends on the impact parameter which determines the deflection angle of the ion in the collision, identified in the second task. As the ion changes direction and transfers energy to the target atom, its velocity components and energy must be recalculated in the last step. Based on the new ion properties, the next free path length is determined and the process is repeated. We will first consider the theory of two atom scattering in the upcoming section and will conclude by discussing the statistics of the free path length distribution to connect individual scattering events to a full trajectory simulation.

2.1.2. Theory of elastic two atom scattering

For small separations r of projectile and target nucleus, the electron shells of both atoms can be neglected and the bare nuclear charge is seen by the projectile nucleus. With larger separations, the electrons begin to screen the nuclear charge and the potential starts to deviate from the classical Coulomb potential

$$V_C(r) = Z \cdot e/4\pi\varepsilon_0\ r. \tag{1}$$

There are different approaches to calculate the electron density of the atomic shell and to derive a screened Coulomb potential $V(r)$. Examples for well-known potentials are the Thomas-Fermi potential approximated by Sommerfeld [14] and the Lenz-Jensen potential [15]. Moliere later derived another potential [16] which is based on the Thomas-Fermi model of the atom [11,12]. The potentials are usually described by a screening function

$$\Upsilon = \frac{V(r)}{V_C(r)} = \frac{V(r)}{Z \cdot e/4\pi\varepsilon_0\ r} \tag{2}$$

by which the Coulomb potential needs to be multiplied. For many potentials, the argument r of the screening function is scaled with the so called screening length a, a variable describing the extent of the electronic shell with a dependency on the nuclear charge Z. This simple formalism reduces the problem to a single screening function which can be used for all kind of atoms just by changing its screening length with the atomic number Z.

For the potential between two atoms, the interaction of the two electronic densities need to be taken into account. Historically, this was solved by introducing a new screening length which averages over both atomic numbers Z_1 and Z_2. Different kind of averages were suggested by Lindhard et al. [17], Firsov [18] and Ziegler et al. [19].

The two body elastic scattering problem we will look at is characterized by the impact parameter p, which is the initial transverse distance of projectile and target (Fig. 2). The problem can be reduced to a one body scattering off the potential $V(r)$ in the center of mass system (CM), as long as the force only acts along the distance of the nuclei. The angle $\phi(p)$ by which the projectile is scattered in the CM system then only depends on the impact parameter p, the potential $V(r)$, and the initial CM energy E_{CM}. Because of the cylindrical symmetry involved, the differential cross section for this event is equal to

$$d\sigma = 2\pi\ p\ dp. \tag{3}$$

Expressed as a differential cross section for scattering into the interval $d\phi$ of angles around ϕ this relation becomes