CALCULATION OF NUCLEAR STOPPING POWER

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ABSTRACT. Fast charged particles interact with matter mainly by interaction with the electron shell of the atoms causing ionization and excitation, i.e. inelastic scattering. However, for lower velocity projectiles an important part of the energy loss is due to elastic scattering on the nuclei, which is called nuclear stopping. In the present paper we calculate the nuclear stopping cross section of protons and antiprotons in different materials. The obtained results are compared with calculations by other groups and with the electronic stopping cross sections. The difference between the results for protons and antiprotons is explained.

Keywords: interaction of charged particles with matter, nuclear stopping, Barkas effect

INTRODUCTION

The interaction of fast charged particles with matter is studied since the discovery of radioactivity. Shortly after the structure of the atom was clarified by the experiments proposed by Rutherford [1], a theory for the slowing down of α and β -rays in matter was published by Bohr [2]. After the elaboration of quantum mechanics, Bethe deduced a formula (based on the Born approximation) for the stopping power of fast ions in matter [3], which is widely used till today.

The slowing down of protons and heavier ions in different materials has great practical importance in many fields. Precise calculations are needed for hadron therapy, different material science and astrophysical applications.

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Charged particles passing through matter lose their energy due to the interaction with the atoms. The most important and extensively studied process is the energy loss of the projectile due to the interaction with the electrons causing excitation or ionization. The mentioned Bethe model considers only this process. However, there exists also energy loss because of the elastic collisions of the projectile with the nuclei. This is negligible relative to the electron stopping at high energies but may be important for lower energy projectiles. This nuclear stopping is far less studied in the literature relative to the electron stopping. Examples of such calculations for proton and other ion projectiles are in the book of Ziegler, Biersack and Littmark [4] and the computer code developed by them [5]. A detailed study for nuclear stopping of antiprotons in different materials was published by Nordlund [6], and some results for helium and hydrogen targets are also available [7, 8].

THEORY

The nuclear stopping is due to the elastic collision of the projectile with the nuclei from the target. Except for extremely low energies, when the de Broglie wavelength of the projectile ion becomes comparable with the atomic dimensions, the collision process may be treated classically. From the theory of classical scattering one obtains, that the θ scattering angle for a projectile with energy E_0 can be written as [7]

$$\theta(b) = \pi - 2 \int_{r_{min}}^{\infty} \frac{b \, dr}{r^2 \sqrt{1 - V(r)/E_c - b^2/r^2}},\tag{1}$$

where b represents the impact parameter of the projectile, r is the distance between the projectile and the target atom (with respective masses m_p and m_t), $E_c = \frac{E_0 m_t}{m_p + m_t}$ is the center-of-mass energy and V(r) is the screened Coulomb potential. The r_{min} distance is given by the largest root for the zero value of the term under the square root.

The energy transferred to the atom during elastic scattering depends on the scattering angle of the projectile:

$$T(b) = 4 \, \frac{m_p \cdot m_t}{(m_p + m_t)^2} \, E_0 \sin^2\left(\frac{\theta}{2}\right).$$
(2)

The nuclear stopping cross section is defined as the integral of the kinetic energy transferred to the target atom over all impact parameters [7],

$$S_n = 2\pi \int_0^\infty b T(b) \, db. \tag{3}$$

The stopping power is related to the stopping cross section by

$$-\frac{\langle \Delta E \rangle}{\Delta x} = N(-S), \tag{4}$$

where N is the atomic density of the target material; the minus sign indicates energy lost by the projectile and transferred to the target atom [9].

If in the expression (2) of the transferred energy one calculates the angle from the pure Coulomb scattering on the nucleus, a divergent integral for the nuclear stopping cross section is obtained, due to the infinite range of the Coulomb potential. In order to avoid this problem one has to take into account the screening effect of the electron cloud, resulting in a projectile-atom potential of finite range.

There are several different models for the calculation of the interaction potential V(r). We have performed the calculations first assuming a frozen electron cloud (more appropriate for fast projectiles), and then a static potential, accounting for the static influence of the projectile on the atom (adiabatic approximation).

For hydrogen, we compare the results calculated from the frozen core model with those obtained with the static potential. For helium we use only the frozen core model, while for Be, C, N, O, Ne, Al and Si targets we use the potential calculated for the antiproton projectile [6] for both proton and antiproton projectiles.

The antiproton projectiles can collide with the nucleus due to the attractive potential, in which case nuclear reactions may occur [6]. Because we did not consider these processes, events where the antiproton came closer than 3 fm to the nucleus were excluded from the calculation. Since the probability of a nuclear reaction is very small, the results do not change significantly.

In the expression of the scattering angle, the value of the integrand approaches infinity near r_{min} , so here we have used an analytical approximation for the first small interval.

RESULTS AND DISCUSSION

Helium

For helium, we calculated the interaction potential applying the frozen core approximation. The potential for proton projectiles, using a wavefunction for the helium atom obtained from a simple variational method, can be written as:

$$V(r) = e^{-2\alpha r} \left(2\alpha + \frac{2}{r} \right), \tag{5}$$

where $\alpha = \frac{27}{16} \approx 1.6875$.

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In Fig. 1, we present our results for the antiproton-helium and proton-helium nuclear stopping cross sections. For antiprotons we find good agreement with the theoretical results of Bailey et al. [9], and Schiwietz et al. [10], respectively for protons with the results of the SRIM program [5]. In both cases, the value of nuclear stopping is found to exceed that of electronic stopping at low energies.

Comparing the results for proton and antiproton projectiles one may observe that the nuclear stopping cross section for antiproton projectiles is significantly higher than for protons, so the Barkas effect [11] is valid also for the nuclear stopping. This result is different from the pure Coulomb scattering, where the cross section does not depend on the charge sign of the projectile. The cause of this charge dependence is that the antiproton, attracted by the nucleus, passes it at a smaller distance, resulting in a higher potential and energy transfer.



Fig. 1: Stopping cross sections (S_n – nuclear, S_e – electronic, S - total) of antiprotons (left panel) and protons (right panel) in He as a function of projectile energy. The present frozen core approximation results are compared to other theoretical calculations: nuclear stopping cross sections of Bailey et al. [7] and Schiwietz et al. [10], electronic and total stopping cross sections of Bailey et al. [7], Borbély et al. [9] and Schiwietz et al. [10], and to the experimental data for \bar{p} of Agnello et al. [8]. For p the electronic and nuclear cross sections obtained from the SRIM program [5] are presented.

Hydrogen

For hydrogen targets, we have calculated the nuclear stopping cross section using both models: the frozen core approximation and using the potential calculated for hydrogen in [6]. The interaction potential calculated from the frozen core model for proton projectile is

$$V(r) = e^{-2r} \left(1 + \frac{1}{r} \right).$$
 (6)

Whereas the adiabatic potential calculated for antiprotons [6] can be written as

$$V(r) = \frac{Z_1 Z_2}{r} \phi^{exp},\tag{7}$$

where ϕ^{exp} is the screening function, which can be written as the sum of a few exponential functions.

In Fig. 2, we present our results for the antiproton-hydrogen and protonhydrogen nuclear stopping cross sections calculated from both the frozen core and adiabatic approximation models. The results calculated for the antiproton from the two models show a significant discrepancy at 10 eV. Since the frozen core model does not take into account the distortion of the electron cloud due to the interaction with the projectile, the value calculated using the adiabatic approximation may be closer to the true nuclear stopping in this case. Our results are lower than the results presented in the article [6]. The reason for the discrepancy may be due to differences in the calculation methods.

For proton projectiles, the adiabatic approximation and frozen core models show good agreement at higher energies, but at lower energies the frozen core model results in a larger stopping cross section than the one calculated with the adiabatic approximation. The adiabatic approximation results are in good agreement with the nuclear stopping cross sections obtained from the SRIM program.



Fig. 2: Stopping cross sections (S_n – nuclear, S_e – electronic, S - total) of antiprotons (left panel) and protons (right panel) in H as a function of projectile energy. The present frozen core and adiabatic approximation results are compared to other theoretical calculations: nuclear stopping cross sections of Nordlund et al. [6] and Schiwietz et al. [10], electronic cross sections of Bailey et al. [7] and Schiwietz et al. [10], and to the experimental data for \bar{p} of Agnello et al. [8]. For p the electronic and nuclear cross sections obtained from the SRIM program [5] are presented.

Silicon

In Fig. 3, we compare our result for the nuclear stopping cross section obtained with the adiabatic approximation for a silicon target with the results of Nordlund et al. [6] and those obtained from the SRIM program. As in the case of hydrogen, there is a discrepancy between the nuclear stopping calculated for antiprotons and the results presented in [6]. The value of nuclear stopping in this case exceeds the value of electronic stopping below 100 eV.

For protons (except for 1 keV), our results are in good agreement with the results of the SRIM program and the results of Nordlund et al. [6].



Fig. 3: Stopping cross sections (S_n – nuclear, S_e – electronic) of antiprotons (left panel) and protons (right panel) in Si as a function of projectile energy. The present adiabatic approximation results are compared to other theoretical calculations: the nuclear cross sections of Nordlund et al. [6] and the data obtained from the SRIM program [5]. The experimental data are taken from [6].

Beryllium

In Fig. 4, we present our results for the antiproton-beryllium and protonberyllium nuclear stopping cross sections calculated from the adiabatic approximation model.



Fig. 4: Stopping cross sections (S_n – nuclear, S_e – electronic) of antiprotons (left panel) and protons (right panel) in Be as a function of projectile energy. The present adiabatic approximation results are compared to other theoretical calculations: nuclear stopping cross section of Nordlund et al. [6] for \bar{p} and the electronic and nuclear cross sections obtained from the SRIM program [5].

There is a significant discrepancy between our results calculated for antiproton projectiles below 100 keV and the results of the article [6]. However, for proton projectiles our results show good agreement with the results of the SRIM program.

Nitrogen

In Fig. 5, we present our results for the antiproton-nitrogen and protonnitrogen nuclear stopping cross sections calculated from the adiabatic approximation model. For antiproton projectiles below 5 keV, there is no good agreement between our results and the results of the article [6]. The values of the proton-nitrogen nuclear stopping cross section are in good agreement with the results of the SRIM program at higher energies, but below 5 keV there is a visible difference between the two curves.



Fig. 5: Stopping cross sections (S_n – nuclear, S_e – electronic) of antiprotons (left panel) and protons (right panel) in N as a function of projectile energy. The present adiabatic approximation results are compared to other theoretical calculations: nuclear stopping cross section of Nordlund et al. [6] for \bar{p} and the electronic and nuclear cross sections obtained from the SRIM program [5].

CONCLUSIONS

Nuclear stopping power of charged particles was studied using a classical model. We have numerically calculated the nuclear stopping cross section of proton and antiproton projectiles for H, He, Be, C, N, O, Ne, Al, and Si targets.

Due to the attractive interaction between the nucleus and the antiproton, the minimal distance between the target and the projectile is smaller, resulting in larger scattering angle and larger energy transfer than for a proton projectile under similar conditions. Thus, for all targets, the nuclear stopping power is higher for antiproton projectiles than for protons of the same energy (Barkas effect). It was shown that at low energies, the value of the nuclear stopping cross section is significant, and in may cases larger, relative to the electronic stopping cross section.

For helium and hydrogen targets we have used a frozen core approximation, and the results obtained were in good agreement with the results of Bailey et al. [7] and Schiwietz et al. [10]. In the case of hydrogen, the small difference with the results of Schiwietz et al. [10] can be explained with the fact that in [10] the nuclear stopping was calculated for hydrogen molecules.

Our results calculated with the Nordlund static potential are not in good agreement with the results presented in the original article [3]. The reason for the discrepancy may be due to differences in the calculation methods. In [6] the interaction of the antiproton with the atoms was modelled by using molecular dynamics simulations. We calculated the nuclear stopping cross sections using equations (1)-(3) with great attention to the convergence of the integrals, which is a more direct method.

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