

Large nuclear scattering effects in antiproton transmission through polymer and metal-coated foils

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We simulate the deceleration and transmission of antiprotons with keV-scale kinetic energies through polymer foils using a molecular dynamics (MD) approach, which includes a model of nuclear stopping based on the attractive interaction potentials between antiprotons and target atoms calculated by quantum chemical methods. Antiprotons scatter into larger angles with higher cross sections than protons. This causes a significant fraction of antiprotons to annihilate in the foil instead of emerging with energies of a few keV, especially when coatings of materials with high atomic number are applied to the surfaces. The simulation results are in good agreement with data from two experiments that involved pulsed antiproton beams with incident energies between 63 keV and 122 keV that traverse polymer foils with thicknesses of $\approx 1.3 \mu\text{m}$ and $1.8 \mu\text{m}$. The 25 nm-thick layers of Ag on the latter foil reduced the transmission of antiprotons. The results will be utilized to design the degrader foils in laser spectroscopy experiments of antiprotonic helium atoms and experiments involving Penning traps that are carried out at the ELENA facility of CERN.

I. INTRODUCTION

The slowing down of ions with keV to MeV per nucleon kinetic energies in solids is conventionally described by the electronic S_e and nuclear S_n stopping powers [1–8]. The former corresponds to the deceleration of the ions by exciting or ionizing the electrons of the target atoms [4–7], whereas the latter arises from the elastic collisions of the ions with the atomic nuclei that are screened by the core electrons. The total stopping power is taken as the sum $S = S_e + S_n$ [6–8], though changes in the interatomic forces caused by electronic excitation and ionization may give rise to couplings or synergetic effects between elastic and inelastic processes that cannot easily be handled by this simple separation [9–13]. While the electronic stopping powers of protons and antiprotons in materials are equal ($S_e^p \approx S_e^{\bar{p}}$) at kinetic energies E_k above a few MeV, at lower velocities the proton value becomes greater ($S_e^p > S_e^{\bar{p}}$) [14–40] which constitutes the Barkas effect [41, 42]. The electronic stopping powers increase rapidly as the proton or antiproton slows down, eventually reaching maxima at around $E_k = 100$ keV in many materials (see Fig. 1). At still lower energies the electronic stopping power decreases linearly with the particle velocity v , while the ratio $R(v) \equiv S_e^{\bar{p}}/S_e^p$ decreases to ≈ 0.5 [20–23].

The nuclear stopping power $S_n^{\bar{p}}$ of antiprotons, on the other hand, is difficult to measure because an elastic col-

lision with a massive atom typically involves only a small reduction in the energy of the antiproton accompanied by a large scattering angle θ that changes the direction of its movement (Figs. 2(a)–(b)). The electronic stopping power including the contributions of ionization processes at low velocities have large theoretical and experimental uncertainties [29–37, 43–45], and thus it is difficult to isolate the nuclear stopping power $S_n^{\bar{p}}$ which is often assumed to be very small. Nevertheless it has been predicted that the $S_n^{\bar{p}}$ contribution is larger than the value for protons and becomes an important energy-loss mechanism at $E_k \leq 1$ keV (Fig. 1) [28, 29, 46–48]. Past theoretical [28–33, 47] and experimental [46, 49] studies of the nuclear stopping power have primarily concentrated on H, H₂, or He gas targets.

Antiprotons arriving with small impact parameters relative to an atom follow complex trajectories that curve toward the nucleus with larger scattering angles θ (see Fig. 2(a)) and cross sections [48] compared to protons that are deflected in the opposite direction along approximately hyperbolic trajectories in the repulsive proton-nucleus potential [28, 29]. Similarly to the kinematics in elastic neutron moderation, the antiproton tends to lose the largest kinetic energy ΔE per elastic collision with a target of similar mass, such as a hydrogen atom (Fig. 2(b)). Collisions with heavier atoms involve larger cross sections and scattering angles, but lower ΔE -values that are kinematically allowed [48]. An experimental indication of $E_k = 1$ –10 keV antiprotons reflecting off of an Al wall [50] has been interpreted in terms of consecutive Rutherford scatterings with multiple scattering angles between 10° and 40° . Depending on the target

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material, the deceleration process at energies of a few hundred eV or less include dominant contributions from some multi-electron and molecular effects that are less understood [45, 51, 52]. The antiproton eventually replaces one or more atomic electrons and forms an antiprotonic atom with \AA^2 -scale cross sections [53–57]. The atom then undergoes electromagnetic cascade processes [58] which leads to the antiproton being absorbed into the nucleus and annihilating.

In-flight annihilation [59–73] constitutes a separate process in which an antiproton with keV-scale or higher energy encounters a nucleus and annihilates without forming an exotic atom. In the semiclassical black-disk model [66–69, 74–76] which is believed to hold for target nuclei of large mass number A and an approaching antiproton of sufficiently short wavelength, the cross section of annihilation may be calculated as,

$$\sigma_A = \pi R^2 \left(1 + \frac{Ze^2(m_{\bar{p}} + M)}{4\pi\epsilon_0 E_k R M} \right). \quad (1)$$

Here the masses of the antiproton and nucleus are respectively denoted by $m_{\bar{p}}$ and M , the vacuum permittivity by ϵ_0 , and the electric charge by e . The effective radius R is assumed to be largely independent of E_k . At energies below a few MeV, the Coulomb potential of the nucleus of charge number Z substantially curves the antiproton trajectory towards the nucleus so that the cross section increases and becomes roughly proportional to $ZA^{1/3}$.

We recently developed a molecular dynamics (MD) [77] approach in the Recoil Interaction Approximation (RIA) [78–80] to model the nuclear stopping powers for several atomic targets allowing simulations of the movement of keV antiprotons in solids [48, 81]. The method is based on the interaction potential between antiprotons and atoms calculated by quantum chemical methods. This yielded a numerically intensive [82], but more precise way of simulating the effects of nuclear stopping and scattering on antiproton motion in solid targets.

In this work we show that the results of MD-RIA simulations are in good agreement with two sets of experimental data involving the transmission of antiprotons with incident energies between 63 keV and 122 keV through polymer foils, within the experimental uncertainties. The prolongation of the pathway of the antiprotons due to the nuclear scattering into large angles that naturally arises as part of our treatment of $S_n^{\bar{p}}$ is found to significantly affect the transmission. Even a thin (≈ 25 nm thick) layer of material with high atomic number such as Ag or Au deposited on the exit surface of the polymer foil was found to reduce the yield of the antiprotons emerging with energies of a few keV.

The Extra Low ENergy Antiproton (ELENA) storage ring [83, 84] provides antiproton beams of 100 keV to several experiments that study antihydrogen [85–92], antiprotonic helium atoms ($\bar{p}^4\text{He}^+ \equiv \bar{p} + ^4\text{He}^{2+} + e^-$) [93–99], and the magnetic moment and cyclotron frequency of antiprotons confined in Penning traps [100–102]. Some

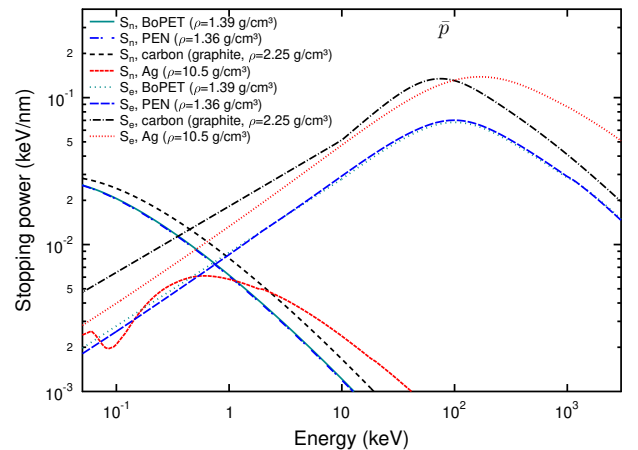


FIG. 1. (color online). Electronic $S_e^{\bar{p}}$ and nuclear $S_n^{\bar{p}}$ stopping powers of antiprotons in BoPET, PEN, C, and Ag targets used in the MD-RIA simulations. The nuclear stopping of Ag has structures at low energy due to the complicated trajectories in the attractive interatomic potential [48]. These $S_n^{\bar{p}}$ values were calculated by integrating the energy transfer ΔE (see Fig. 2) that was obtained by MD simulations of antiproton collisions with single atoms. At kinetic energies of a few hundred eV or less depending on the target atom or molecule, the cross section for an antiproton replacing one or more electrons and forming an antiprotonic atom are predicted to reach values of \AA^2 scale [46, 51–53]. This contribution is not included in this figure which is based on an adiabatic Born-Oppenheimer approximation that allows the separation of $S_e^{\bar{p}}$ and $S_n^{\bar{p}}$.

of these experiments involve slowing down the antiprotons to energies $E_{\text{trans}} \leq 5 - 10$ keV by allowing them to pass through foils of 1 μm -scale thicknesses [90–92]. The antiprotons can then be efficiently captured in the electrostatic potential of a Penning trap of typical depth of 5–10 kV. In other experiments the antiprotons are allowed to come to rest in gas targets of low density to form antiprotonic atoms in which the rates of collisions with the surrounding atoms are minimized. Such collisions may shift or broaden the measured spectral energies [103–107], cause the recapture of electrons by the antiprotonic atoms [108], or shorten the state lifetimes [58, 109, 110]. In some past experiments involving Penning traps, 5.3 MeV antiprotons provided by the Antiproton Decelerator (AD) [111–113] were slowed down in foils that were up to 10^3 times thicker. The stochastic nature of the straggling [23, 114–116] in the electronic stopping due to the large number of collisions caused $\approx 99.8\%$ of the antiprotons to annihilate in the foils before they could emerge at keV energies. The lower energy and momentum spread $\Delta p/p \approx 10^{-3}$ of the ELENA beam are designed to reduce this loss of antiprotons [83, 84]. This paper analyzes the effects of foil material and thickness on the antiproton deceleration and transmission.

The paper is organized in the following way. Two ex-

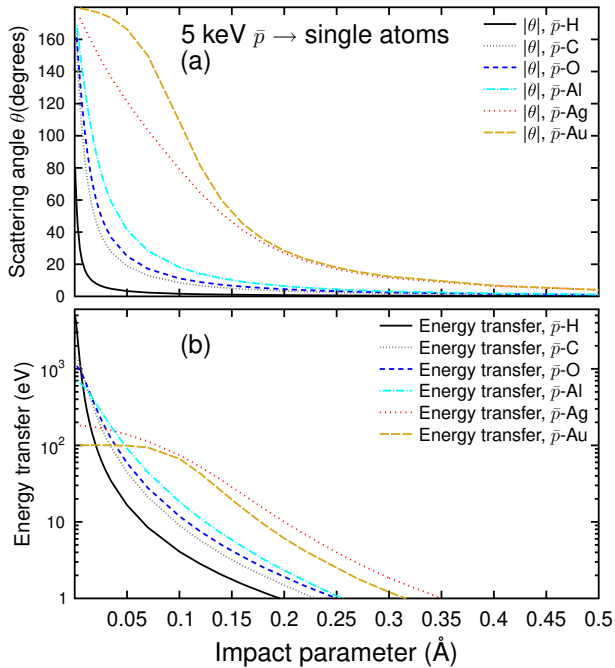


FIG. 2. (color online). (a) Scattering angle θ and (b) kinetic energy transfer ΔE in the laboratory frame of an elastic collision between an antiproton of incident energy $E_k = 5$ keV and a H, C, O, Al, Ag, or Au atom as a function of the impact parameter b . The energy transfer for Ag and Au are kinematically limited to $\Delta E = 100$ and 200 eV, respectively, by the reduced mass of the system and E_k . The values were obtained using MD simulations of collisions between an antiproton and each target atom that were based on the antiproton-atom potentials. The maximum impact parameters that lead to annihilation were $b_A \approx 0.001$ \AA and 0.004 \AA for C and Au targets, respectively (see Fig. 6).

periments that involve the slowing down of antiprotons in polymer foils, namely the laser spectroscopy experiment of $\bar{p}^4\text{He}^+$ and some measurements using a Penning trap [91], are described in Sections II A and II B, respectively. The models of nuclear and electronic stopping powers used in the simulations are outlined in Sections III A and III B. Some details of the MD-RIA simulation are provided in Section III C. The transmission probabilities and energy distributions of the antiprotons emerging from the foils obtained from MD-RIA, GEANT4, and SRIM2013 simulations are compared with the experimental results in Section IV. The effects of various experimental conditions were included in the simulation in a stepwise manner. Some discussions and conclusions are provided in Section V.

II. EXPERIMENTAL METHODS

A. Laser spectroscopy of $\bar{p}^4\text{He}^+$

We utilized laser spectroscopy of $\bar{p}^4\text{He}^+$ [95, 96] to determine the relative numbers of antiprotons that were transmitted through a polyethylene naphthalate (PEN) foil of nominal thickness $t_r = 1300$ nm. The foil acted as a hermetically-sealed window of a cryogenic helium gas target and withstood a differential pressure of 100 Pa. PEN consists of H, C, and O atoms that causes less nuclear scattering during the transmission of the antiprotons compared to heavier atoms.

The three-body $\bar{p}^4\text{He}^+$ atom consists of a helium nucleus, an electron in the 1s state, and an antiproton occupying a Rydberg state with large principal and angular momentum quantum numbers $n \approx \ell + 1 \approx 38$. For this experiment the AD provided a $\Delta t \approx 150$ ns long pulsed beam containing some $(2 - 3) \times 10^7$ antiprotons of energy 5.3 MeV at a repetition rate of 0.008 Hz. The antiprotons entered a radiofrequency quadrupole decelerator (RFQD) [117–119] which contained four 3.4-m long rod electrodes excited at a frequency of 202.6 MHz to produce a maximum electric field of 33 MV/m. A (20–25)% fraction of the antiprotons that matched the longitudinal acceptance of the device emerged with a nominal energy $E_{\text{nom}} = 63$ keV, emittance of $> 50 \pi$ mm mrad, and 1 standard-deviation energy spread $\sigma_E \approx 5$ keV. The remaining antiprotons either passed through the RFQD with incomplete deceleration or struck the RF electrodes and were not used. The average energy of the slow antiprotons was varied between $E_{\text{nom}} - V_{\text{bias}} = 63$ keV and 122 keV by biasing the RFQD with a DC potential between $V_{\text{bias}} = 0$ kV and -59 kV. The antiprotons were then diverted by an achromatic momentum analyzer that was connected to the output of the RFQD, and focused into a $d \approx 15$ mm-diameter spot at the entrance of a helium gas target. The spatial profiles of the beam at three locations along the beamline were measured by secondary electron emission detectors consisting of wire electrodes [120]. The relative intensity of the beam was measured by a lead fluoride Cherenkov detector [121].

The antiprotons traversed the PEN window and came to rest in a chamber filled with ^4He gas having a pressure of ≈ 100 Pa and temperature $T \approx 1.5$ K. This resulted in the formation of $\bar{p}^4\text{He}^+$. At a time $t \approx 8 \mu\text{s}$ after the formation, a 40 ns long laser pulse with a diameter of 50 mm and a pulse energy of 2 mJ was fired into the chamber in a counter-propagating direction to the antiproton beam [122]. The laser wavelength of 264.7 nm was tuned to excite a transition between a $\bar{p}^4\text{He}^+$ resonance parent state $(n, \ell) = (32, 31)$ with a 1 μs -scale lifetime, and a daughter state $(31, 30)$ that led to Auger emission of the electron with a lifetime of ≈ 3 ns. The $\bar{p}^4\text{He}^{2+}$ ions that remained were destroyed by collisions with other helium atoms in the target [123, 124]. The sharp increase in the flux of charged pions that emerged from the antipro-

ton annihilations was detected by an acrylic Cherenkov detector [125]. The intensity of the signal was proportional to the number of atoms that were irradiated by the laser beam, and the population occupying the parent state (32, 31) corresponding to $\approx 10^{-3}$ of the number of antiprotons that came to rest in the helium gas [58]. The signal indicating the transmission of antiprotons through the foil was measured as a function of the beam energy.

These measurements were repeated using eight foils of the same nominal thickness over a period of 8 years [95, 96], and the reproducibility of the E_k dependence was found to be distributed over ± 5 keV in terms of incident energy. The average thicknesses of two of the foils were measured using a Rutherford backscattering technique [69, 126] and found to be within $\pm 10\%$ of the nominal values which roughly agrees with the values reported by other authors [127]. Prior to the measurements, the foils were evacuated to a pressure of between 10^{-6} Pa and 10^{-7} Pa at room temperature for several days to reduce the contamination on their surfaces. The foils were then cooled to $T \leq 1.5$ K and the spectroscopy experiments were carried out. Thin layers of contamination gradually froze on the foil surfaces over time so that the transmission of the antiprotons was affected. The contamination was removed by heating the foil to room temperature.

B. Antiproton Penning trap

The second set of experimental results were obtained using a Penning trap [90] as reported in Ref. [91]. We here describe the experimental details that are relevant for the comparison with the simulations. The beam emerging from the RFQD entered the bore of a superconducting solenoidal magnet of field $B = 2.5$ T. The antiprotons traversed a pair of biaxially-oriented polyethylene terephthalate (BoPET) foils with nominal thickness $t_r = 900$ nm which constituted the position-sensitive cathodes of a beam profile monitor, before being captured within the cylindrical electrodes of the trap with a total length of ≈ 700 mm and an inner diameter of 40 mm. A (25 ± 3) nm-thick layer of Ag was deposited on the front surface of each BoPET foil by vacuum evaporation. Patterns of ten 0.94 mm-wide electrode strips with a 1 mm pitch between neighboring strips were then fabricated on the Ag surfaces using a laser trimmer [120, 128]. The pair of patterned foils were stacked with the two Ag electrode surfaces that provided the horizontal and vertical projections of the beam facing outwards. The material layers were thus arranged in the sequence Ag, BoPET, and Ag with thicknesses $t_r = 25$ nm, 1800 nm, and 25 nm, respectively. Antiprotons traversing the electrodes induced secondary electron emission. By measuring the corresponding charge signal induced on each electrode strip with a charge-sensitive preamplifier, a full-width-at-half-maximum beam diameter of 2–3 mm was observed [91].

The relative intensity of annihilations in the foils at beam energies between $E_k = 92$ keV and 122 keV was

measured by a Cherenkov detector [125] which was placed outside the solenoidal magnet. In a separate measurement, antiprotons of average incident energy $E_k = 111.5$ keV traversed the foils and travelled along the axis of the solenoid, before reaching a plate located $l > 1.5$ m away outside the magnetic bore. By scanning the electrostatic potential applied to an electrode of the trap and measuring the relative intensity of the annihilations on the plate, the energy distribution E_{trans} of the antiprotons that emerged from the foil were determined. The Ag coatings developed pinholes over several years [129] which may alter the transmission properties.

III. SIMULATION METHOD

A. Nuclear stopping model

1. Simulation models of nuclear stopping

In many models of nuclear stopping, the trajectory of each ion in the target is tracked to simulate the effects of nuclear scattering which alter the direction of the ion movement. In the binary collision approximation (BCA) [8, 130, 131] the pathway of the positively-charged ion is separated into a series of isolated two-body collisions with the target atoms. The ion follows a hyperbolic trajectory in the repulsive potential of the atom, but BCA employs computationally-efficient methods to determine the straight ion pathway that is asymptotic to the actual hyperbola for each collision [131, 132]. The electronic stopping S_e contribution slows down the ion in the straight pathways between the collisions. The SRIM2013 code [8, 133] utilizes the Monte Carlo variant of BCA, in which after each collision the impact parameter b relative to the next target atom is stochastically chosen according to a probability distribution. SRIM2013 does not, however, allow the simulation of antiprotons since the code is based on calculating the asymptotes of hyperbolic trajectories [132], whereas negatively-charged particles that are deflected inwards toward the nucleus within an attractive potential follow more complicated trajectories [48].

The GEANT4 code [134] has been used to simulate the passage of MeV to GeV antiprotons through materials for many years. The cumulative effects of a large number of collisions and scatterings into small angles that occur within an ion trajectory segment of given length are here approximated by one of several multiple scattering models that may be selected by the user [135–140]. The computations involved in these so-called “condensed” simulations are vastly reduced compared to the MD method that explicitly solves the equations of motion for every collision that the ion undergoes (see below). We used the Wentzel-VI multiple scattering model [135, 138–141] implemented in GEANT4 version 10.7 to simulate the antiproton scatterings into smaller angles. The code separately calculated the contributions of nuclear scattering events into larger angles by using a single elastic scatter-

ing model. This model was based on the Wentzel scattering function [135, 142] with the same shape as the one used in the above multiple scattering model. The electronic stopping power $S_e^{\bar{p}}$ of antiprotons was modeled by treating the atoms as an ensemble of quantum harmonic oscillators [15, 39, 143–145].

The molecular dynamics in the recoil interaction approximation (MD-RIA) method, by comparison, models ions and atoms moving under arbitrary interatomic forces [77, 146, 147]. This allows antiproton scatterings that occur in the attractive antiproton-atom potentials of multiple atoms comprising the lattice to be explicitly and more precisely simulated [48, 78–81]. The MD [77, 148] method follows the atomic motion over time in short ($\lesssim 0.1$ Å) spatial steps in an iterative and deterministic way by calculating the sum of all the forces exerted from the neighbouring atoms. The contributions of multiple simultaneous collisions that can increase the energy transfer ΔE compared to the results of BCA at ion energies of $\lesssim 1$ keV are thus inherently included. The method does not rely on any assumption regarding the specific scattering model, trajectory shape, or collision strength. In the recoil interaction approximation, only the interactions between the projectile ion and target atoms are evaluated, whereas the interactions between the lattice atoms that would vastly increase the computation are neglected [78].

2. Interaction potentials

We calculated the interaction potentials between antiprotons and Cu, Ag, and Au atoms that include the contributions of atomic screening functions using the method of Ref. [48]. Density functional theory (DFT) calculations provided the interaction energy between the antiproton (treated as a negative point charge surrounded by the basis functions of the hydrogen atom) and a Cu, Ag or Au nucleus surrounded by its 29, 47 or 79 electrons, respectively. The interaction energy as a function of the distance between the atomic nucleus and the antiproton was calculated at 48 discrete points in the range between $r = 0.0001$ bohr and 50 bohr using version 7.5 of the Turbomole code [149–151]. The calculations were performed at the DFT level with the range-separated ω B97X-D functional in the meta-generalized gradient approximation (mGGA) using grid 7, which is a dense integration grid [152, 153]. The Cu atomic orbitals were expanded in a decontracted triple- ζ polarization (def2-TZVP) basis set, whereas for the antiproton a decontracted hydrogen def2-TZVP basis set was utilized [154]. For the Ag atom, a decontracted Turbomole all-electron TZVP basis set (TZVPPalls2) was used. For the Au atom, we used the relativistic exact two-component (X2C) Hamiltonian and the decontracted x2c-TZVPPall Au basis set [155, 156]. The corresponding level of theory was used in the nonrelativistic calculations on Au. These interaction energies are provided in Appendix A.

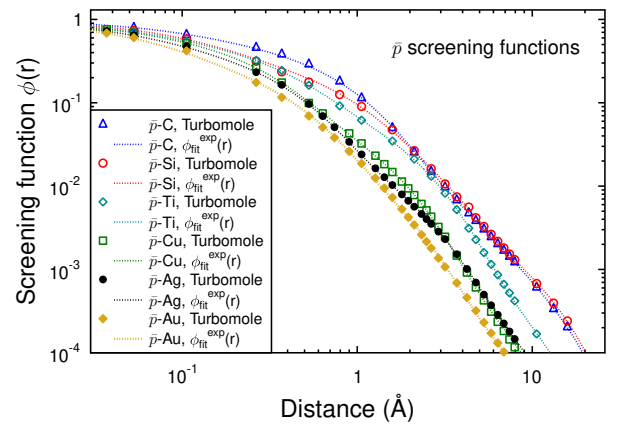


FIG. 3. (color online). The results of the best fit of the screening function $\phi_{\text{fit}}^{\text{exp}}(r)$ of Eq. 3 on the interaction potentials between an antiproton and C, Si, Ti, Cu, Ag, or Au atom. The C, Si and Ti functions are reproduced from Ref. [48].

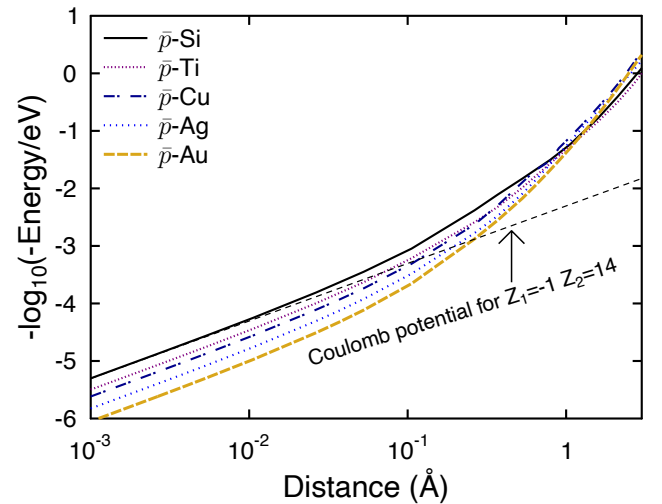


FIG. 4. (color online). Interaction potentials between an antiproton and target Si, Ti, Cu, Ag, and Au atoms calculated by quantum chemical methods. The Si and Ti potentials are reproduced from Ref. [48]. The bare Coulomb potential for an antiproton and Si atom is also shown for comparison.

The calculated data were fit to a Coulomb potential with an exponential screening term of the form,

$$V(r) = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2 e^2}{r} \phi(r). \quad (2)$$

Here $Z_1 = -1$, Z_2 , and e denote the antiproton, nuclear, and elemental charges, respectively. The screening term $\phi(r)$ was taken to have the exponential form [48],

$$\phi_{\text{fit}}^{\text{exp}}(r) = b_1 e^{a_1 r} + b_2 e^{a_2 r} + b_3 e^{a_3 r} + b_4 e^{a_4 r}. \quad (3)$$

The coefficient of the last term is defined as $b_4 \equiv 1 - b_1 - b_2 - b_3$ which ensures that the potential of Eq. 2 has a pure

Coulomb form at short distances, i.e., $\phi_{\text{fit}}^{\text{exp}}(r \rightarrow 0) = 1$. Fig. 3 shows the calculated screening functions of the Cu, Ag, and Au atoms, together with those of C, Si, and Ti obtained previously [48]. The parameters b_i and a_i determined by the best fit of Eq. 3 to the calculated antiproton-Si, -Cu, -Ag, and -Au interaction potentials are summarized in Table I. The potentials involving Si, Ti, Cu, Ag, and Au atoms are shown in Fig. 4.

In Figs. 2(a)–(b), the scattering angle θ and energy transfer ΔE for an elastic collision between an antiproton of incident energy $E_k = 5$ keV and a single isolated H, C, O, Al, Ag, or Au atom in the above potentials are shown as a function of impact parameter b . The results were obtained using a MD simulation of binary collisions between an antiproton and a single atom. The trajectories with impact parameters of less than $b_A \approx 0.001$ Å and 0.004 Å for the C and Au targets, respectively, approach within a few femtometers of the nucleus [69, 76, 157]. These trajectories were removed from Figs. 2(a)–(b) based on a simplified approximation (labeled as model B in Section III A 4) of the effects of antiproton annihilations.

3. Nuclear stopping curve

The nuclear stopping powers $S_n^{\bar{p}}$ of antiprotons in atomic C, H, O and Ag targets were calculated by integrating the energy transfer ΔE over the impact parameter b . The Bragg averaging rule [1, 8] was then applied to the results to obtain the $S_n^{\bar{p}}$ values in the PEN and BoPET foils. These were found to be approximately equal (Fig. 1) and slightly smaller than the values for a pure C target of graphite density. As the antiprotons slow down from an energy of 10 keV to less than 1 keV, the $S_n^{\bar{p}}$ values increase from ≈ 1 eV/nm to more than 10 eV/nm, eventually becoming larger than the electronic stopping powers which decrease from $S_e^{\bar{p}} \approx 30$ eV/nm to less than 10 eV/nm over the same energy range. The nuclear stopping power of Ag is larger than those of the polymeric materials at energies above a few keV. As the antiproton slows down, the ΔE -value becomes kinematically limited so that a saturation at $S_n^{\bar{p}} \approx 5$ keV/nm is seen.

4. Antiproton annihilation

The atoms in our MD-RIA simulations were fixed to the electronic ground states throughout the collisions. The contributions of some complex electronic processes that occur at energies of a few hundred eV or less, such as the antiproton replacing the atomic electrons and forming antiprotonic atoms [51–57] or effects involving electronically-excited or ionized states of the target atom are therefore not included.

In most of the simulations, we instead modelled the nuclear absorption of antiprotons using a simplified and computationally efficient approach, henceforth called an-

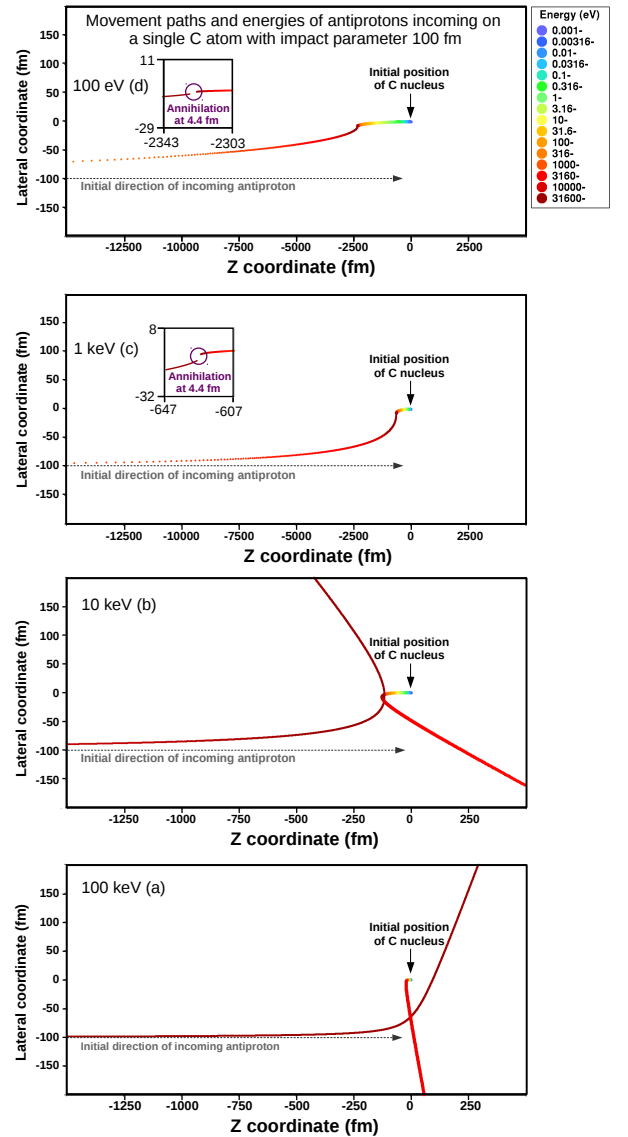


FIG. 5. (color online). Trajectory of an antiproton with an impact parameter $b = 100$ fm and incident energy $E_k = 100$ keV (a), 10 keV (b), 1 keV (c), or 100 eV (d) scattering off a single C atom positioned at the origin calculated by MD-RIA. Note the different horizontal and vertical scales. The gradients indicate the kinetic energies of the antiproton and C atom in logarithmic scale. Annihilations occur when the antiproton comes within $\langle r_A \rangle = 4.4$ fm of the C atom [76] (see inserts). As the antiproton accelerates when approaching the nucleus, the integration steps in time are reduced to ensure the numerical stability of the results [78].

nihilation model A. The kinetic energy of the antiproton is evaluated throughout the collision with multiple atoms and during the deceleration due to the electronic stopping power. When this energy becomes smaller than the absolute value of the local interaction potential $|\phi(r)|$, the antiproton is taken to orbit the nucleus and annihilate. Though in-flight annihilation that occurs at higher ener-

TABLE I. The values of the coefficients b_i and a_i of the antiproton screening function $\phi_{\text{fit}}^{\text{exp}}(r)$ of Eq. 3 that were obtained by the best fit on the calculated potentials between an antiproton and a Si, Cu, Ag, or Au atom. The coefficient of the last term is defined as $b_4 \equiv 1 - b_1 - b_2 - b_3$ to ensure that the potential is of a pure Coulomb form with bare nuclear charges at short length scales $r \rightarrow 0$. The parameters for Si are obtained from Ref. [48].

Target	b_1	b_2	b_3	a_1	a_2	a_3	a_4
Si	0.00547494	0.360324	0.091372	-0.19811	-1.99426	-0.79267	-9.71705
Cu	0.00176877	0.715859	0.106417	-0.333232	-5.1509	-1.28497	-27.2726
Ag	0.000985221	0.563975	0.0374024	-0.260267	-3.91193	-0.944955	-19.0258
Au	0.000854978	0.400538	0.0380799	-0.322095	-3.86192	-1.21461	-17.2175

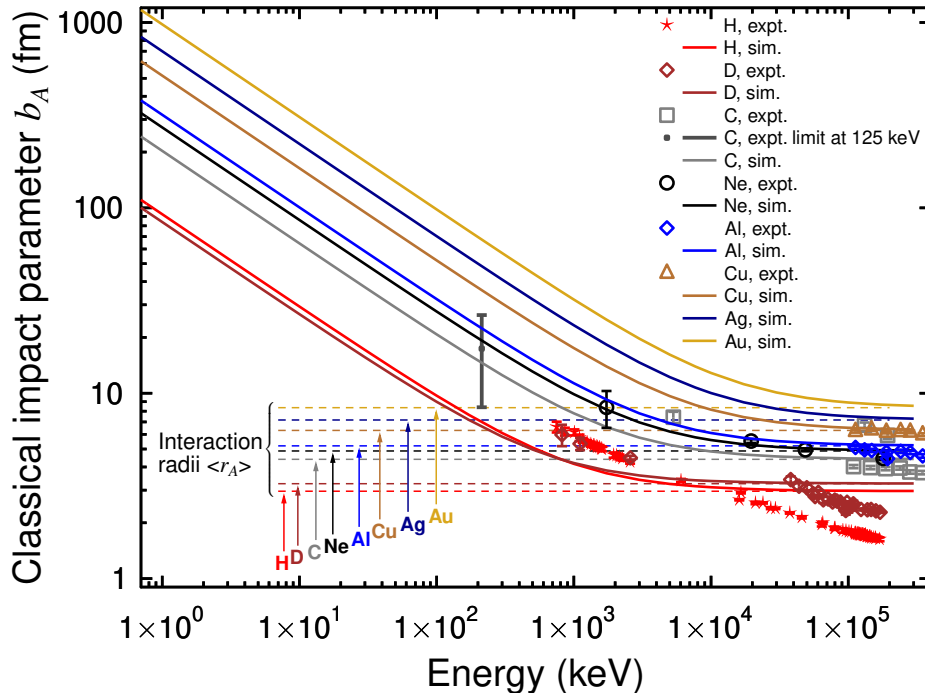


FIG. 6. (color online). Minimum impact parameter b_A of an antiproton colliding with a H, D, C, Ne, Al, Cu, Ag, or Au atom that leads to in-flight annihilation as a function of the incident energy E_k calculated using MD-RIA. The simulations utilized the average interaction radii $\langle r_A \rangle$ according to Eq. 4 [76] shown in the figure for each target. The experimental values of H [59–62], D [63–65], C [68, 70], Ne [71, 72], Al, and Cu [70, 73] targets that were obtained from the measured annihilation cross sections σ_A and assuming the relation $\sigma_A = \pi b_A^2$ are shown superimposed. The vertical line with error bars for C at $E_k = 125$ keV represents the experimental limit of Ref. [69]. The curves are arranged in the same sequence as in the indicated labels.

gies are ignored, this model is sufficient to evaluate the fraction of the antiprotons transmitted through the foils.

In some of the MD-RIA simulations a more complex model B that takes both the in-flight annihilations and the capture of low-energy antiprotons into account was used. In this model annihilation occurs when the antiproton comes within the effective interaction radius r_A of the nucleus which is taken to be independent of the incident energy E_k . This black disk model is believed to be valid for massive target nuclei with diameters that are sufficiently large compared to the wavelength of the antiproton [66, 74, 76]. We used the average interaction radius,

$$\langle r_A \rangle = 1.840 + 1.120(A)^{1/3} \text{ fm}, \quad (4)$$

that was derived from the unified optical potential model of Ref. [76]. Eq. 4 was obtained by folding the optical potential of the antiproton-proton system that was obtained from experiments carried out at $E_k \approx 750$ keV, with the matter density distributions of the nuclei. Comparisons with the results of x-ray spectroscopy experiments of antiprotonic atoms with mass number $A > 10$ have shown that the model reproduces the shifts and widths of the atomic energy levels that arise due to the strong interaction [76]. These spectroscopy measurements effectively study the antiproton-nuclei scattering at nearly zero energy.

The simulated trajectories of antiprotons with impact parameter $b = 100$ fm and incident energies $E_k = 100$ keV and 10 keV that scatter off C atoms are shown in

Figs. 5(a) and (b), respectively. At lower energies $E_k = 1$ keV (Fig. 5(c)) and 100 eV (Fig. 5(d)), the more pronounced curvature of the trajectories allow the antiprotons to approach the nuclei within the $\langle r_A \rangle = 4.4$ fm distance implied by Eq. 4 and annihilate.

Fig. 6 shows the values of the maximum impact parameter b_A that leads to annihilation in H, D, C, Ne, Al, Cu, Ag, and Au nuclei that were determined in this way. Antiprotons of high energy ($E_k \gtrsim 5$ MeV) approach the nuclei along straight trajectories so that the impact parameter b_A is roughly equal to $\langle r_A \rangle$. At lower energies, the focusing effect of the Coulomb force causes b_A to rapidly increase. The results were compared with the experimental cross section σ_A of antiproton annihilations which were taken to relate to the impact parameter as $\sigma_A = \pi b_A^2$. The lack of experimental data at energies below a few MeV makes this comparison difficult, but the simulation and experimental results are consistent for C [68–70], Ne [71, 72], Al, and Cu [70, 73] targets within the experimental uncertainties. Deviations are seen in H [59–62] and D [63–65] for which the semiclassical parameterization of Eq. 4 is not expected to be a good approximation. Indeed, partial-wave decomposition analysis [158, 159] have shown that the cross sections for these light nuclei at low energies are dominated by the contributions of the s - and p -wave components of the approaching antiproton. The fraction of $E_k = 1$ –100 keV antiprotons that undergo in-flight annihilation is relatively small (see below), as the corresponding b_A values of approximately 10–1000 fm are 2–4 orders of magnitude smaller than the interatomic distances of ≈ 100 pm.

B. Electronic stopping

We developed a generalized expression for the electronic stopping power $S_e^{\bar{p}}(v)$ of antiprotons to deduce the values in atomic targets for which experimental data were not available. The procedure was based on our observations (see Fig. 7) that the generalized stopping ratio $R(v) \equiv S_e^{\bar{p}}(v)/S_e^p(v)$ between the experimental antiproton and proton stopping powers in C, Si, and Al targets [20] are equal over a range of antiproton velocities v within the experimental uncertainties. This is because the S_e values at low projectile velocities are approximately proportional to the electron density in the target [160, 161]. We used the exponential parameterization,

$$S_e^{\bar{p}}(v) = R(v)S_e^p(v) = \left(1 - R_g e^{-v/v_g}\right) S_e^p(v), \quad (5)$$

to reflect the experimental fact that at high velocities the electronic stopping powers of protons and antiprotons become approximately equal, i.e., $R(v \rightarrow \infty) = 1$. The best fit on the experimental data for C, Al and Si targets yielded values of $R_g = 0.6105 \pm 0.013$ and $v_g = (7.95 \pm 0.62) \times 10^6$ m/s for the two constants. The largest systematic deviations (Fig. 7) in the experimental data sets used in the fitting were -6% for the C data, and

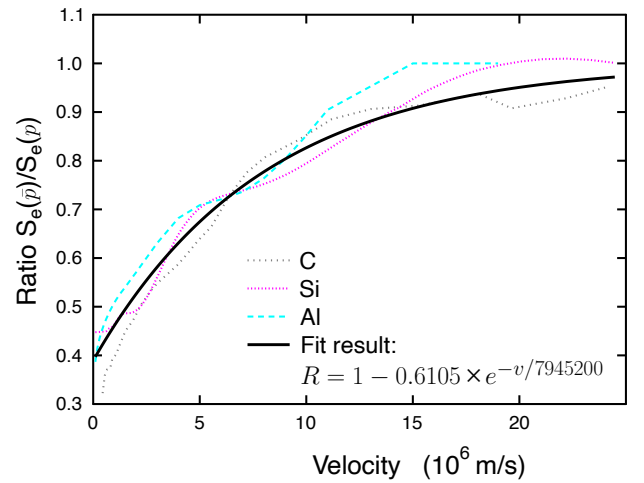


FIG. 7. (color online). The generalized electronic stopping ratio $R(v)$ as a function of the velocity of the antiproton and proton. The dashed curves indicate the ratios $S_e^{\bar{p}}/S_e^p$ between the experimental antiproton [20] and proton stopping powers in C, Si and Al targets. The solid curve shows the result of the best fit of the indicated exponential function.

7% for Al. As the antiproton-atom interactions that are involved in the nuclear scattering do not follow a simple scaling relation relative to the proton-atom interactions, a similar scaling procedure could not be employed to deduce the nuclear stopping powers $S_n^{\bar{p}}$.

Fig. 8 compares the electronic stopping powers of antiprotons in Cu, Ag, and Au targets that were estimated using the scaling procedure of Eq. 5 with the experimental data [20, 21]. The agreement is particularly good for the Au target at energies between $E_k \approx 7$ keV and 100 keV, which indicates that the model is valid over a wide range of atomic targets. At higher energy regions deviations of up to 15% that are comparable with the fluctuations in the experimental data are seen. These electronic stopping powers together with those of BoPET, PEN, graphite, and Ag targets shown in Fig. 1 were used in the MD-RIA simulations.

C. Simulation setup

The MD-RIA code MDRANGE [78, 162] was used to simulate the transmission of antiprotons through a homogeneous PEN ($C_{14}H_{10}O_4$) foil of thickness $t_r = 1300$ nm, or three sequential layers of Ag, BoPET ($C_{10}H_8O_4$), and Ag with $t_r = 25$ nm, 1800 nm, and 25 nm, respectively, that were utilized in the experiments. Simulations were also carried out for foils with Al, Cu, or Au coatings of the same thicknesses. The PEN and BoPET materials were modelled as $2 \times 2 \times 2$ nm³ cubes containing atoms with the above elemental ratios and densities of 1.36 g/cm³ and 1.38 g/cm³, respectively. As the materials lack any long-range order, the atoms were distributed at random-

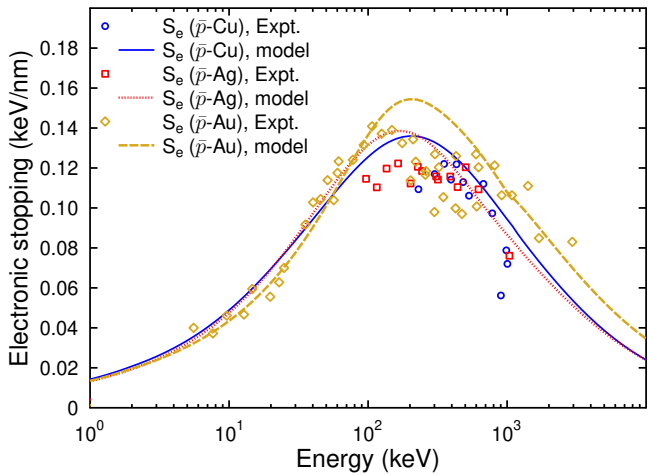


FIG. 8. (color online). Electronic stopping powers $S_e^{\bar{p}}$ of antiprotons in Cu, Ag, and Au targets obtained from the generalized scaling method, compared with experimental data [20, 21].

ized locations with a minimum interatomic distance of 1.1 Å. The evaporated coatings were modelled as amorphous structures with the densities shown in Table II, as they were nanocrystalline with random surface orientations. As the channeling effects of keV antiprotons even in single crystals are predicted to be small [48], the simulation results were not significantly affected by the small cell size or the partial order in the polymeric materials. We included the electronic stopping power $S_e^{\bar{p}}(v)$ and straggling [114–116] in each foil layer. Past simulations of the transmission of $E_k = 4$ keV protons through C foils have found that the straggling must be included to obtain a good agreement with experimental data [163].

The antiprotons arrived in a perpendicular direction to the foil surface with an energy spread that was taken to be Gaussian with a standard deviation $\sigma_E = 5$ keV to simulate the properties of the RFQD beam. The initial lateral positions of the antiprotons were randomized over a 1×1 nm² area at the center of the $2 \times 2 \times 2$ nm³ cubic cell to ensure an uniform sampling over different trajectories through the compound materials [48]. A few thousand random numbers that defined the initial positions and energies of the antiprotons were generated using the Mersenne twister [164] with a repeat period of $2^{19937} - 1$. The positions of the atoms were randomly shifted to simulate the thermal motion [165], but this had a negligible effect on the results for these amorphous materials. Between 10^3 and 10^5 trajectories were simulated to determine the energies and angles of the antiprotons that traversed the foil for each condition. The contributions of the nuclear stopping and scattering were isolated by comparing the results with other simulations (indicated as “ S_e only” in the figures) in which the interparticle potential and forces were set to zero so that the slowing down was only due to the electronic stopping.

IV. RESULTS

A. Fractions of transmitted antiprotons

1. Comparison with experiments

Fig. 9(a) presents the relative intensity of the antiproton beam that traversed and emerged from the 1300 nm-thick PEN foil as a function of the incident energy E_k (indicated by filled squares), which was measured by laser spectroscopy of $\bar{p}^4\text{He}^+$ [95, 96]. Only the antiprotons that came to rest in the volume of the helium gas irradiated by the laser beam contributed to the signal. The results are therefore expected to be relatively insensitive to the trajectories of the antiprotons that exited the foil. A good agreement between the experimental and MD-RIA results (blue solid curve) is seen within the systematic uncertainties of the foil thickness (see below). The curve calculated by removing the nuclear stopping contribution is shifted to lower energies by 30 keV compared to the experimental data. Antiprotons that exited with a large off-normal angle θ_{exit} may stop outside the area irradiated by the laser beam and avoid detection. We took this possible effect into account by rejecting the simulated antiprotons with $\theta_{\text{exit}} > 50^\circ$. This slightly improved the overall agreement between the simulation (blue dotted curve) and experimental results.

Fig. 10(a) shows the results of the Penning trap experiment in which the fraction of antiprotons that annihilated in the Ag-coated BoPET foil or in its vicinity instead of being transmitted, was measured as a function of the beam energy. A good agreement with the MD-RIA results (blue solid curve) is seen except at the highest energy $E_k = 122$ keV. The reason for this difference is not understood. Our simulations did not include the effects of the uniform magnetic field of $B = 2.5$ T that was applied in the direction normal to the foil surface [91]. In the experiment, on the other hand, the antiprotons that emerged with a lateral velocity component v_\perp perpendicular to the normal of the foil surface underwent cyclotron motion with an approximate Larmor radius,

$$r_{\text{Larmor}} = \frac{m_{\bar{p}} v_\perp}{eB}. \quad (6)$$

Antiprotons with large radii eventually struck the inner walls of the trap or other electrodes that were located at the exit end of the solenoidal magnet [91]. The simulation results (blue dotted curve) obtained by assuming that the antiprotons with $r_{\text{Larmor}} > 5$ mm annihilated and contributed to the signal is in better agreement with the experimental result at $E_k = 122$ keV. When the effects of nuclear stopping and scattering $S_n^{\bar{p}}$ are removed, the simulation results (grey dotted curve) shift to lower energies by a factor of 1.5–2 in terms of E_k .

The results of the GEANT4 simulation (Fig. 9(b)) for $E_k < 80$ keV overestimate the transmission probability through the 1300 nm-thick PEN foil compared to the experimental data. A relatively good agreement is seen in

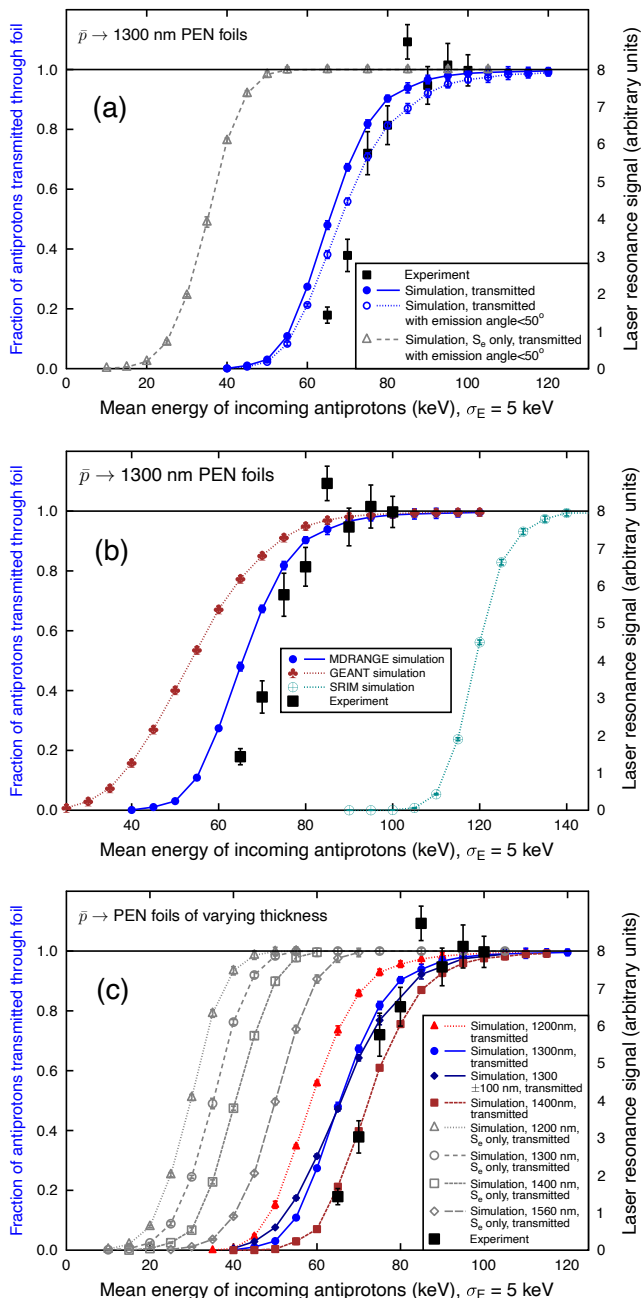


FIG. 9. (color online). (a) Relative intensities (filled squares) of antiprotons transmitted through a 1300 nm-thick PEN foil measured by laser spectroscopy of $\bar{p}^4\text{He}^+$ as a function of the incident beam energy. The results of MD-RIA simulations with (filled circles) and without (open triangles) the nuclear scattering and stopping S_n , and the curve obtained by selecting the antiprotons that exit the foil with an angle $\theta_{\text{exit}} < 50^\circ$ (open circles) are shown superimposed. (b) Simulation results for antiprotons of the MDRANGE and GEANT4 codes, and the proton result of SRIM2013. (c) Fractions of antiprotons that emerged from PEN foils of uniform thicknesses $t_r = 1200$ nm, 1300 nm, 1400 nm, and 1560 nm simulated with and without the $S_n^{\bar{p}}$ contribution. The results of a simulation in which the foil thickness was varied around the average value of 1300 nm by a standard deviation $\sigma_t = 100$ nm are also shown.

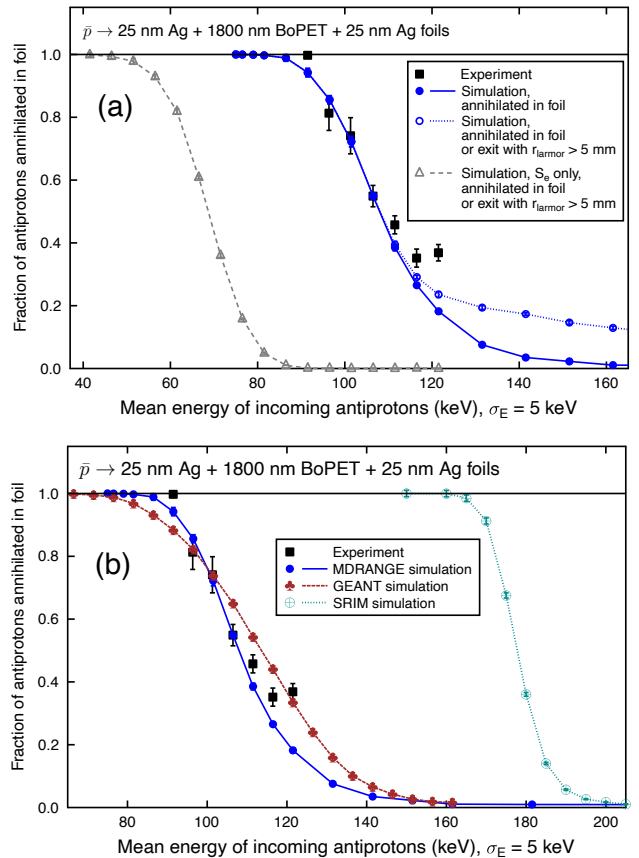


FIG. 10. (color online). (a) Experimental fractions of antiprotons (filled squares) [91] that annihilated in the BoPET foil instead of being transmitted, as a function of the incident energy E_k . The results of simulations with (filled circles) and without (open triangles) the nuclear stopping $S_n^{\bar{p}}$ contribution, and by assuming that the antiprotons that exited the foil with a Larmor radius $r_{\text{Larmor}} > 5$ mm rapidly annihilate (open circles). (b) Comparisons with MDRANGE and GEANT4 simulation results for antiprotons, and the proton result of SRIM2013.

the case of the $E_k \geq 100$ keV antiprotons traversing the Ag-coated BoPET foil (Fig. 10(b)). These simulations did not include the discrimination involving the Larmor radius and exit angle.

As SRIM2013 cannot handle antiprotons we used it to calculate the transmission of protons. The results (see Figs. 9(b) and 10(b)) were nearly identical to those of MDRANGE. Proton energies that are a factor 1.5–1.7 greater than for antiprotons are needed to traverse the foils because of the larger electronic stopping power.

2. Effects of foil thickness variation

The transmission probabilities of the antiprotons through PEN foils of uniform thicknesses $t_r = 1200$ nm, 1300 nm, 1400 nm, and 1560 nm that were calculated

with and without the nuclear stopping $S_n^{\bar{p}}$ contribution are compared in Fig. 9(c). A change of ± 100 nm in t_r was found to shift the transmission probability curves by $\pm(5 - 7)$ keV in terms of the incident beam energy E_k . The curve corresponding to $t_r = 1400$ nm best agrees with the experiment. We next introduced random variations in the thickness across the foil surface which corresponded to a standard deviation $\sigma_t = 100$ nm around the nominal value $t_r = 1300$ nm. Similar thickness or equivalent density variations in BoPET foils have been reported by other authors [127]. The variation slightly flattened the shape of the transmission probability curve.

B. Energy distributions of transmitted antiprotons

1. Comparisons with MD-RIA, GEANT4, and experiments

Fig. 11(a) presents the measured and simulated energy distributions E_{trans} of antiprotons emerging from the 1800 nm-thick BoPET foil with Ag coatings used in the Penning trap experiment, for an average beam energy of 111.5 keV and energy spread of 5 keV [91]. The simulation results are normalized to the total number of incident antiprotons including those that stop in the foil, whereas the experimental data are normalized using the measured fractions of antiprotons that annihilated in or near the foil as shown in Fig. 10(a). The agreement between the MD-RIA and experimental results improves when the effects of nuclear stopping $S_n^{\bar{p}}$ are included. The experiment detected few antiprotons of $E_{\text{trans}} \leq 3$ keV. This may partially be due to the slow antiprotons that followed complex trajectories in the magnetic field and annihilated in the solenoidal magnet without being detected. Preliminary measurements at ELENA using a different apparatus and beam energy appear to show significant fractions of $E_{\text{trans}} \approx 1$ keV antiprotons.

The energy distribution obtained from the GEANT4 code is in relatively good agreement with the experimental data within the systematic uncertainties. It is peaked more sharply compared to the distribution obtained from MD-RIA.

2. Effects of thickness variation

The energy E_{trans} distributions of the antiprotons traversing BoPET foils of thicknesses $t_r = 1700$ nm, 1800 nm, and 1900 nm with 25 nm-thick Ag coatings are compared in Fig. 11(b). Antiprotons with Larmor radii $r_{\text{Larmor}} > 5$ mm were rejected. The curve for the nominal value $t_r = 1800$ nm best agrees with the experimental results. An uncertainty of ± 100 nm on t_r was found to correspond to a ± 3 keV shift in the peak of the E_{trans} distribution. This shift is significant compared to the 5–10 kV confining electrostatic potential of the Penning trap, implying that a stack of foils having a thickness adjusted with an accuracy of ± 50 nm may be needed to

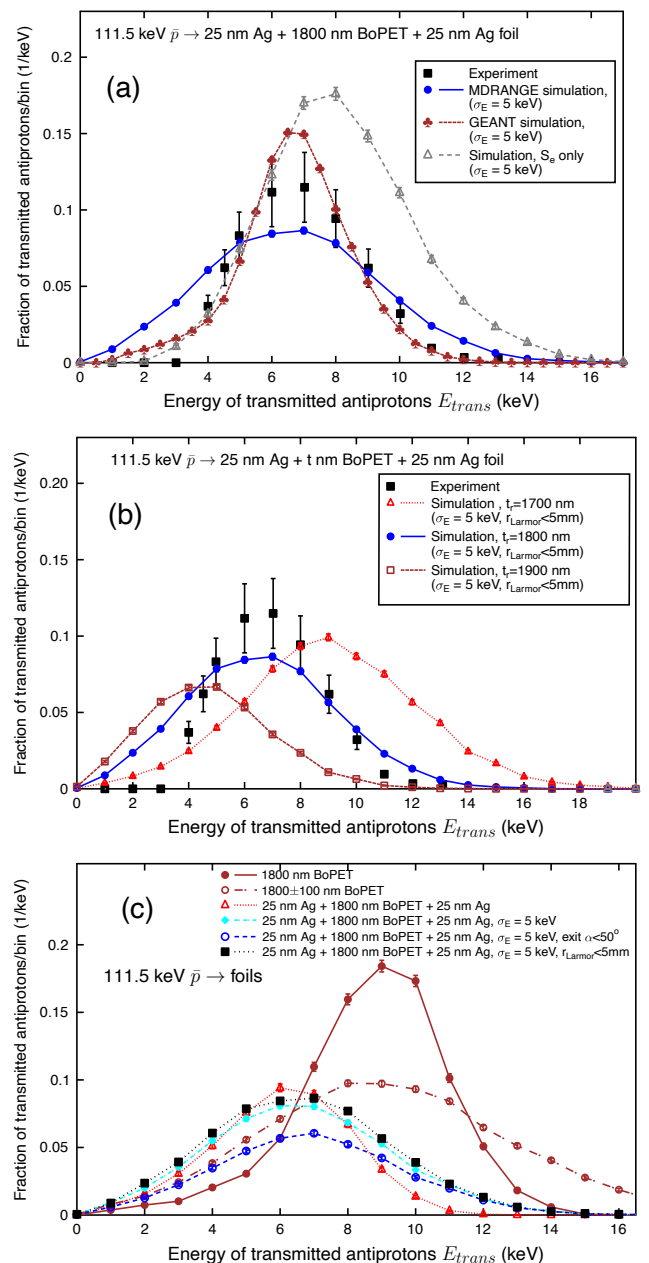


FIG. 11. (color online). (a) Experimental (filled squares) energy E_{trans} distributions of antiprotons that emerge from the 1800 nm-thick BoPET foil with Ag coatings [91] for an incident beam energy of 111.5 keV. The distribution is normalized to the fraction of antiproton annihilations according to Fig. 10. Simulated distributions calculated using MD-RIA with (filled circles) and without (open triangles) the contribution of nuclear stopping, normalized to the total number of incident antiprotons. The results of the GEANT4 code are shown superimposed. (b) Simulated distributions for foils of $t_r = 1700$ nm (open red triangles), 1800 nm (filled circles), or 1900 nm (open squares) with Ag coatings. (c) The distributions for 1800 nm-thick foils with and without Ag coatings, and with a variation of the BoPET thickness $\sigma_t = 100$ nm. The distributions obtained by selecting the antiprotons that exit the foil with an angle $\theta_{\text{exit}} < 50^\circ$ or Larmor radius $r_{\text{Larmor}} < 5$ mm are shown superimposed.

TABLE II. The results of MD-RIA simulations for an antiproton beam with an incident energy of 111.5 keV and energy spread of 5 keV traversing an uncoated BoPET foil, or foils with 25 nm-thick Al, Cu, Ag, or Au coatings with the indicated densities and total thickness of 1850 nm. The average path length R_{path} , electronic energy deposition F_{D_e} , fraction of antiprotons f_{stop} that come to rest in the foil, and average energy $\langle E_{\text{trans}} \rangle$ of the emerging antiprotons are shown. Also indicated are the results for the Ag coating applied to only the entrance (labelled as upstream) or exit (downstream) foil surfaces, and with a hypothetical material Ag* in which the electronic stopping power of Ag is adjusted to be equal to that of BoPET. The models A or B used to simulate the in-flight annihilation and low-energy capture of the antiprotons by the nuclei are indicated. The indicated uncertainties arise from the dispersion of the trajectories.

Coating material	Coated surface	Coating density (g·cm ⁻³)	R_{path} (nm)	F_{D_e} (keV)	f_{stop} (%)	$\langle E_{\text{trans}} \rangle$ (keV)	Annih. model
Uncoated			1859±1	103.8±0.3	12.6±0.3	7.55±0.02	A
Al	Both	2.7	1855±1	104.3±0.5	16.5±0.5	7.21±0.04	A
Cu	Both	9.0	1844±1	105.5±0.5	33.8±0.7	6.76±0.04	A
Ag	Both	10.5	1840±1	105.8±0.4	39.0±0.4	6.69±0.02	A
Ag	Both	10.5	1834±4	106.1±0.2	35.7±2.1	6.48±0.12	B, $\langle r_A \rangle = 4.4$ fm
Ag	Both	10.5	1840±1	106.0±0.1	39.0±0.4	6.69±0.02	B, $\langle r_A \rangle = 10$ fm
Ag	Upstream only	10.5	1861±1	104.5±0.1	17.2±0.5	6.88±0.03	A
Ag	Downstream only	10.5	1839±1	105.1±0.1	32.1±0.6	7.33±0.04	A
Ag*	Both	10.5	1844±1	104.7±0.1	32.3±0.6	7.66±0.04	A
Au	Both	19.3	1830±2	106.3±0.7	53.7±0.9	6.68±0.05	A

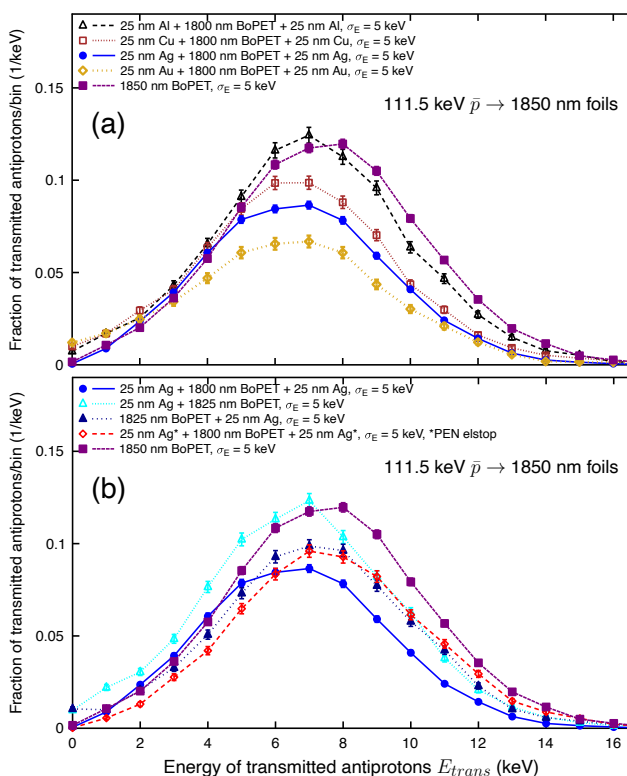


FIG. 12. (color online). (a) Simulated energy distributions of antiprotons emerging from a 1850 nm-thick uncoated BoPET foil, or foils with 25 nm-thick Al, Cu, Ag, or Au coatings applied on both sides. The incident beam energy was adjusted to 111.5 keV with a spread of 5 keV. (b): Distributions calculated for foils with 25 nm-thick Ag coatings applied to the entrance, exit, or both surfaces. The hypothetical case in which the electronic stopping power of Ag is adjusted to be equal to that of BoPET is indicated as Ag*.

trap the maximum number of antiprotons. Alternatively the beam energy E_k may be tuned over a range of ± 10 keV to compensate for the typical uncertainty in the average foil thickness of ± 100 nm.

The distribution for a monoenergetic ($\sigma_E = 0$) beam traversing a 1800 nm-thick BoPET foil is indicated by filled brown circles in Fig. 11(c). A foil with a typical thickness variation $\sigma_t = 100$ nm across its surface (brown open circles) resulted in a reduction in the antiproton yield at the peak of the distribution located at ≈ 9 keV by a factor of ≈ 2 , and a broadening of its width by several keV. The variation must be reduced to $\sigma_t < 20$ –30 nm to avoid this loss in the number of trapped antiprotons.

3. Effects of metallic coatings

When 25 nm-thick Ag coatings were applied to the two sides of the BoPET foil, the antiproton yield at the peak of the E_{trans} distribution (indicated using red open triangles in Fig. 11(c)) decreased by a factor of ≈ 2 and its position shifted from 9 keV to 6 keV compared to the above case of a monoenergetic beam traversing a bare uniform foil. The inclusion of an energy spread $\sigma_E = 5$ keV in the beam further broadened the distribution (blue filled circles) towards higher energies by ≈ 1 keV. Rejecting the transmitted antiprotons with exit angles $\theta_{\text{exit}} > 50^\circ$ (blue open circles) reduced the yield by another $\approx 30\%$, whereas removing those with Larmor radii $r_{\text{Larmor}} > 5$ mm had a relatively small effect (black filled squares). This implied that between 15% and 30% of the incident antiprotons fit into the acceptance of a Penning trap of potential depth 5–10 keV under the experimental conditions of Refs. [90, 91]. Further antiprotons are lost during the subsequent electron cooling in the trap.

Fig. 12(a) compares the E_{trans} distributions for a beam

of $E_k = 111.5$ keV and $\sigma_E = 5$ keV traversing BoPET foils of a total thickness $t_r = 1850$ nm with 25 nm-thick metallic coatings. The fraction of antiprotons that come to rest in the uncoated foil (Table II) was $f_{\text{stop}} \approx 13\%$. This increased to 17%, 34%, 39%, and 54% when Al, Cu, Ag, and Au coatings of incrementally larger atomic number were applied, respectively.

The results for Ag coatings applied on either the upstream (i.e., entrance), downstream (exit), or both foil surfaces are shown in Fig. 12(b). Most of the annihilations occur in the downstream Ag layer through which keV-scale antiprotons are transmitted (Table II). In the hypothetical case in which the electronic stopping power of Ag is adjusted to be equal to that of BoPET (indicated as Ag*), about $f_{\text{stop}} \approx 32\%$ of the antiprotons come to rest in the foil. The fact that this fraction is so similar in the Ag-coated case (39%) shows that the loss of antiprotons is primarily caused by the nuclear scattering into large angles rather than the electronic stopping power. This fact was verified by simulations of $E_k = 5$ keV antiprotons traversing a 25 nm-thick Ag or Ag* foil which showed a stopped fraction $f_{\text{stop}} = 30\%$, whereas for a 25 nm-thick BoPET foil the fraction was 1%.

V. DISCUSSIONS AND CONCLUSIONS

The substantial differences between the simulation results with and without the nuclear stopping contribution may seem surprising, as the $S_n^{\bar{p}}$ values become large only at antiproton energies below about 1 keV (see Fig. 1). This difference arises from the nuclear scattering which increases both the path length of the antiprotons,

$$R_{\text{path}} = \int_{\text{path}} |d\vec{r}|, \quad (7)$$

and the corresponding total deposited electronic energy,

$$F_{D_e} = \int_{\text{path}} S_e^{\bar{p}} |d\vec{r}|. \quad (8)$$

Table II shows the R_{path} and F_{D_e} values, the stopped fraction f_{stop} , and transmitted energy $\langle E_{\text{trans}} \rangle$ of antiprotons with average incident energy $E_k = 111.5$ keV and energy spread $\sigma_E = 5$ keV traversing BoPET foils with total thicknesses of 1850 nm and various coatings. One of two models of antiproton annihilation described in Section III A 4 was used, namely A): comparing the kinetic energy of the antiproton with the local interaction potential in the material, or B): adjusting the average interaction radius to $\langle r_A \rangle = 4.4$ fm for C atoms according to Eq. 4, or to $\langle r_A \rangle = 10$ fm for all target elements. The transmission probabilities of antiprotons calculated by both models were similar within the statistical uncertainty of the simulations, despite the fact that model A ignores the effect of in-flight annihilations. This is because a collision involving a sufficiently small impact

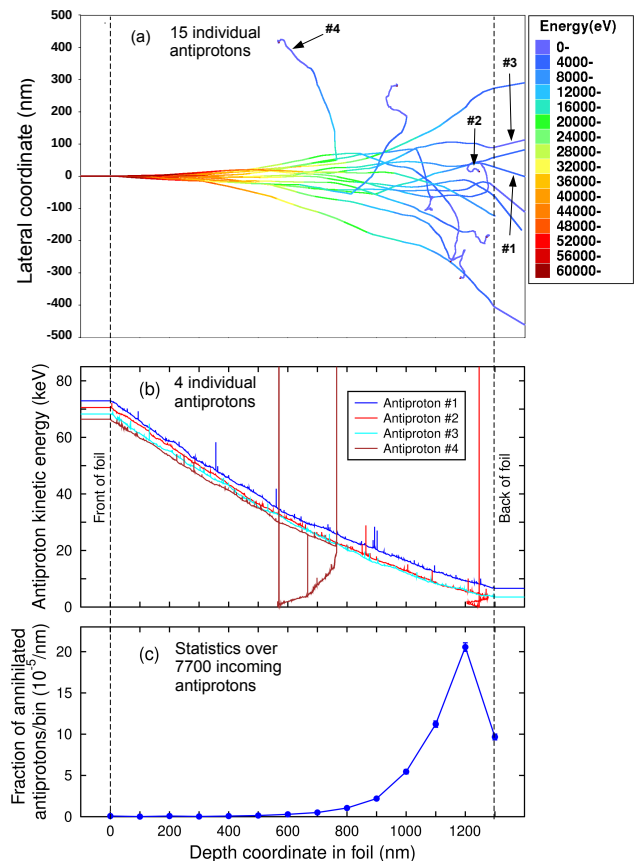


FIG. 13. (color online). (a) Trajectories of 15 antiprotons of incident energy 65 keV and energy spread 5 keV that traverse a 1300 nm-thick PEN foil calculated by MD-RIA. Color gradients indicate the antiproton energy, with the highest energy being on the left side of the figure and the lowest energy being on the right. Each trajectory begins at positions that are slightly laterally shifted. Some 40% of the antiprotons travel through and emerge from the foil. (b) Evolution of the energies of four antiprotons labelled #1 - #4 in (a) projected along the depth coordinate of the foil, with #2 and #4 coming to rest in the foil. The peaks in the energy correspond to antiprotons being attracted by a nucleus during a close collision. (c) Spatial distribution of the antiproton annihilations projected along the depth coordinate.

parameter results in such a large scattering angle θ that the antiproton likely cannot traverse the foil even if it avoids direct in-flight annihilation. This is illustrated in Fig. 13(a) which shows the trajectories of 15 antiprotons of $E_k = 65$ keV and $\sigma_E = 5$ keV in a 1300 nm-thick PEN foil. Fig. 13(b) shows the evolutions of the energies of four of the antiprotons as a function of the depth coordinate along the thickness of the foil. Large-angle scattering and annihilation become more likely as the antiprotons slow down, so that most of the annihilations occur in the last 200 nm-thick portion of the foil (see Fig. 13(c)).

As shown in Fig. 14(a), the path length R_{path} of the cohort of antiprotons that come to rest in the foil in-

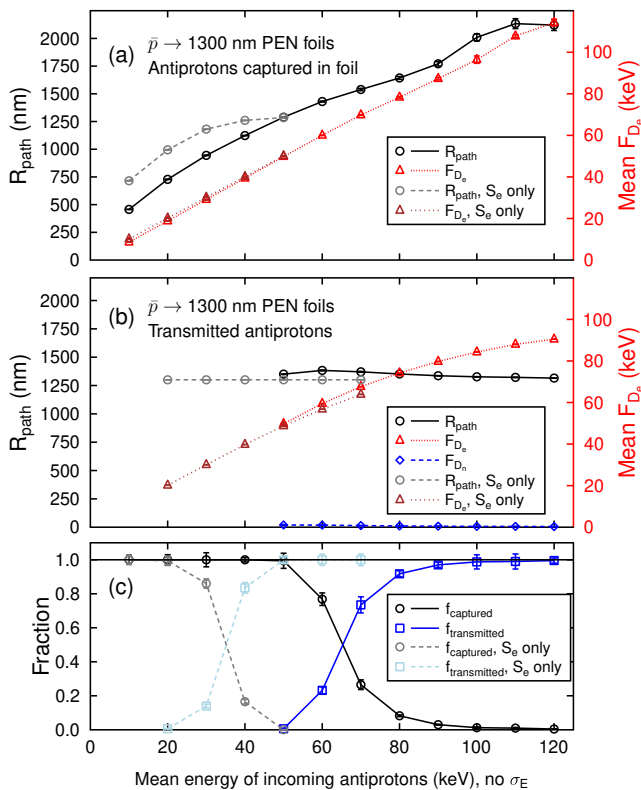


FIG. 14. (color online). Path lengths R_{path} , and total deposited electronic F_{D_e} and nuclear F_{D_n} energies of the cohort of antiprotons that (a) came to rest in, or (b) were transmitted through, a 1300 nm-thick PEN foil as a function of incident beam energy E_k . (c) The probabilities of the antiprotons being transmitted through the foil (indicated as $f_{\text{transmitted}}$) or coming to rest in the foil (f_{captured}). The curves calculated without the contribution of the nuclear stopping power are indicated as “ S_e only”. The simulations were carried out for a monoenergetic beam.

creases with the beam energy. It eventually becomes much longer than the foil thickness of 1300 nm in the region above the minimum incident energy $E_k = 50$ keV that allows antiproton transmission (Fig. 14(c)).

The R_{path} values of the transmitted antiprotons (Fig. 14(b)), on the other hand, remain only slightly longer than the foil thickness regardless of the incident energy between $E_k = 50$ and 120 keV. The deposited electronic energy F_{D_e} increases with E_k , whereas the energy F_{D_n} lost by nuclear stopping remains negligibly small. As shown in Table II, these R_{path} and F_{D_e} values vary by only $\approx 1\%$ for foils with Al, Cu, Ag, or Au coatings, whereas the fraction of stopped antiprotons increases from $f_{\text{stop}} = 17\%$ to 54%. All these results show that the transmitted antiprotons represent the cohort that statistically managed to traverse the foil without undergoing scattering events into large angles.

Fig. 15(a) compares the average energies $\langle E_{\text{trans}} \rangle$ of the cohort of antiprotons that were transmitted through the Ag-coated BoPET foil as a function of incident energy

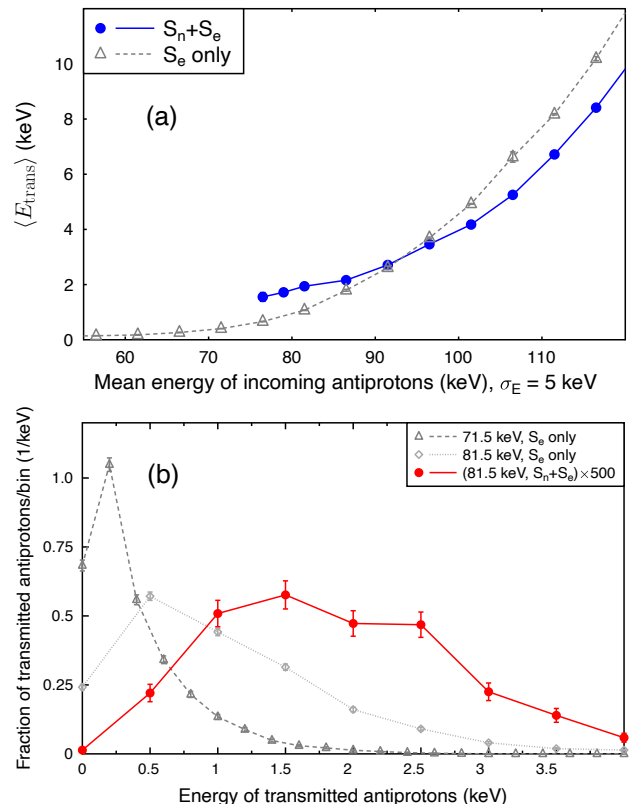


FIG. 15. (color online). (a): Average energy $\langle E_{\text{trans}} \rangle$ of the antiprotons that emerge from the Ag-coated BoPET foil, simulated with (filled circles) and without (open triangles) the contribution of the nuclear stopping power S_n^p . (b): Energy distributions E_{trans} of the emerging antiprotons for incident beam energies $E_k = 71.5$ keV (triangles) and 81.5 keV (diamonds) calculated without the S_n^p contribution. The distribution corresponding to $E_k = 81.5$ keV (circles) that includes the S_n^p contribution multiplied by a factor of 500 is shown superimposed.

E_k , calculated with and without the nuclear stopping contribution. In the region $E_k = 100$ –120 keV the nuclear stopping reduced the $\langle E_{\text{trans}} \rangle$ value by 1–2 keV. We attempted to slow down more antiprotons to $E_{\text{trans}} \leq 1$ keV by reducing the incident beam energy to $E_k = 81.5$ keV. This caused most of the antiprotons to annihilate in the foil (Fig. 15(b)) because of the rapid increase of the nuclear scattering cross section at energies below 2–3 keV (Fig. 1). Further losses are expected due to antiproton capture at sub-keV energies [51, 52]. Alternative methods such as electrostatic drift tubes [166] may be used to efficiently decelerate such slow antiprotons.

In conclusion, we showed that the MD-RIA model of antiproton deceleration in polymer foils which includes the effects of nuclear stopping in antiproton-atom interaction potentials, is in good agreement with experimental results in the sub-100 keV energy region. The significant nuclear scattering predicted by this model was found to

affect the transmission probability and energy distribution of the antiprotons that emerge from the foils, particularly in the energy range below 1–2 keV. Some recent experiments at ELENA have utilized foils with Ag or Au coatings of a few tens nanometer thickness to reduce the thermal radiation entering a Penning trap or the out-gassing of contamination gases, but nuclear scattering in materials of such high atomic number decreases the yield of the transmitted antiprotons. A beam with a small energy spread $\sigma_E < 1$ keV should ideally be slowed down in a uniform foil made of light atoms with a thickness adjusted with a few tens nanometer accuracy. The typical uncertainties of the order of ± 100 nm in the thickness of polymer foils may be compensated by tuning the energy of the incident beam over a range of ± 10 keV. The results will aid the design of experiments to increase the production of antihydrogen and antiprotonic atoms.

The simulation results presented in this paper, the source code of MDRANGE, and the software dpc used to create the trajectory plots are available at [167].

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APPENDIX A. ANTIPROTON-ATOM INTERACTION ENERGIES

The antiproton-Cu, Ag, and Au interaction energies calculated in this work are provided in Table III. The fit result for Au shown in Table I was obtained using the interaction energies that include relativistic corrections that significantly influence the quantum-chemical properties [168]. The nonrelativistic energies are also shown.

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TABLE III. The interaction energy between an antiproton and Cu, Ag, or Au atom calculated using Turbomole. The results of both non-relativistic and relativistic calculations are compared for the Au case.

Distance r (bohr)	Interaction energy			
	Cu (hartree)	Ag (hartree)	Au, non-relativistic (hartree)	Au, relativistic (hartree)
0.0001	-291508.38648833550	-474940.26580643450	-807336.03379621136	-808420.13061681925
0.0002	-146508.37690470659	-239940.23235710687	-412335.95031069889	-413420.08517008071
0.0005	-59508.35241796065	-98940.15187504669	-175335.79833371995	-176420.29541588307
0.0007	-42936.91114894993	-72082.97220379818	-130192.92068154475	-131277.80078712621
0.001	-30508.32615905464	-51940.08496197249	-96335.86359198054	-97421.46500700344
0.002	-16008.32786787354	-28440.19251555596	-56837.04751262472	-57925.74187472051
0.005	-7308.72560386451	-14342.09923704072	-33146.21240693634	-34245.28667918866
0.007	-5652.12163430147	-11658.59451289787	-28640.47188096082	-29745.52939401055
0.01	-4410.38144802696	-9648.44700629965	-25268.70047621010	-26380.85066817488
0.02	-2965.61295330282	-7314.47676463869	-21361.30830037316	-22486.02582377577
0.05	-2112.53034330175	-5941.93490798830	-19067.72183993740	-20204.50467965725
0.07	-1955.42417871681	-5689.43626613219	-18650.90630308088	-19791.92134002133
0.1	-1840.64679008272	-5506.51919531918	-18352.60638631582	-19496.42261014716
0.2	-1715.62679076727	-5311.73807909679	-18037.86592366084	-19185.08545412219
0.5	-1656.06317420202	-5222.04771594475	-17898.18282732744	-19046.85016222893
0.7	-1647.78410291230	-5211.17816304953	-17883.48122363939	-19032.25847588926
1.0	-1643.42474370343	-5204.70978555750	-17875.73970068054	-19024.63050177367
1.2	-1642.34392131365	-5202.86846688449	-17873.52764269468	-19022.48743140719
1.4		-5201.86914678365	-17872.30358104002	-19021.30267979419
1.5	-1641.75553599784			
1.7	-1641.27470464369	-5201.09738470162	-17871.35553309078	-19020.36535962364
2.0	-1641.01393815872	-5200.72134362942	-17870.89823761911	-19019.88937167094
2.4	-1640.82190664246	-5200.47735090297	-17870.60110433715	-19019.56220201497
2.7	-1640.73861799048	-5200.38031981547	-17870.48213868662	-19019.42810139394
3.0	-1640.68442778878	-5200.31888296489	-17870.40693124349	-19019.34369556023
3.4	-1640.63846247687	-5200.26742068708	-17870.34411274284	-19019.27454313786
3.7	-1640.61529498963	-5200.24220817752	-17870.31339520206	-19019.24173851145
4.0	-1640.59825170174	-5200.22403790369	-17870.29129686297	-19019.21887172585
4.4	-1640.58200826146	-5200.20694614383	-17870.27055090209	-19019.19824743790
4.7	-1640.57324751888	-5200.19771706353	-17870.25939300871	-19019.18762567490
5.0	-1640.56658758792	-5200.19058136831	-17870.25086801658	-19019.17981169293
5.5	-1640.55875443201	-5200.18181485256	-17870.24075683928	-19019.17101017777
6.0	-1640.55359565539	-5200.17559103446	-17870.23396470003	-19019.16548317975
7.0	-1640.54775746996	-5200.16771627142	-17870.22557667860	-19019.15914027616
8.0	-1640.54500587156	-5200.16345273919	-17870.22095626702	-19019.15590059917
9.0	-1640.54363919437	-5200.16112865958	-17870.21832141822	-19019.15416606397
10.0	-1640.54291330433	-5200.15983587899	-17870.21674899881	-19019.15318214351
11.0	-1640.54249924987	-5200.15908053792	-17870.21577143232	-19019.15259179284
12.0	-1640.54224769456	-5200.15861169572	-17870.21514194048	-19019.15222122534
13.0	-1640.54208654925	-5200.15830489253	-17870.21472324823	-19019.15197928601
14.0	-1640.54197882723	-5200.15809624241	-17870.21443637177	-19019.15181618795
15.0	-1640.54190433458	-5200.15795013177	-17870.21423476532	-19019.15170262988
20.0	-1640.54174759705	-5200.15763470004	-17870.21379785843	-19019.15146103512
25.0	-1640.54170565339	-5200.15754842050	-17870.21367770981	-19019.15139637311
30.0	-1640.54169080843	-5200.15751717581	-17870.21363460380	-19019.15137321013
35.0	-1640.54168450372	-5200.15750394388	-17870.21361571271	-19019.15136319190
40.0	-1640.54168154486	-5200.15749720351	-17870.21360716906	-19019.15135832053
45.0	-1640.54167996884	-5200.15749393473		
50.0	-1640.54167905724	-5200.15749203100		

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