Nuclear Instruments and Methods in Physics Research B 279 (2012) 92–95

Contents lists available at SciVerse ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Monte Carlo simulation and Boltzmann equation analysis of non-conservative positron transport in H_2

A. Banković [a,*], S. Dujko [a,b,c], R.D. White [c], S.J. Buckman [d], Z.Lj. Petrović [a]

[a] Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
[b] Centrum Wiskunde and Informatica (CWI), P.O. Box 94079, 1090 GB Amsterdam, The Netherlands
[c] ARC Centre for Antimatter–Matter Studies, School of Engineering and Physical Sciences, James Cook University, Townsville, QLD 4810, Australia
[d] ARC Centre for Antimatter–Matter Studies, The Australian National University, Canberra, ACT 0200, Australia

ARTICLE INFO

Article history:
Available online 23 November 2011

Keywords:
Positrons
Hydrogen
Monte Carlo
Boltzmann equation
Transport coefficients
Ps formation
Non-conservative collisions

ABSTRACT

This work reports on a new series of calculations of positron transport properties in molecular hydrogen under the influence of spatially homogeneous electric field. Calculations are performed using a Monte Carlo simulation technique and multi term theory for solving the Boltzmann equation. Values and general trends of the mean energy, drift velocity and diffusion coefficients as a function of the reduced electric field E/n_0 are reported here. Emphasis is placed on the explicit and implicit effects of positronium (Ps) formation on the drift velocity and diffusion coefficients. Two important phenomena arise; first, for certain regions of E/n_0 the bulk and flux components of the drift velocity and longitudinal diffusion coefficient are markedly different, both qualitatively and quantitatively. Second, and contrary to previous experience in electron swarm physics, there is negative differential conductivity (NDC) effect in the bulk drift velocity component with no indication of any NDC for the flux component. In order to understand this atypical manifestation of the drift and diffusion of positrons in H_2 under the influence of electric field, the spatially dependent positron transport properties such as number of positrons, average energy and velocity and spatially resolved rate for Ps formation are calculated using a Monte Carlo simulation technique. The spatial variation of the positron average energy and extreme skewing of the spatial profile of positron swarm are shown to play a central role in understanding the phenomena.

1. Introduction

Positron interactions with matter play important role in many physical processes of interest. Some examples include the origin of astrophysical sources of annihilation radiation [1], the use of positrons in medicine (e.g., positron emission tomography (PET)) [2], the characterization of materials [3], production and detection of cold antihydrogen (the first step in the creation and study of stable, neutral antimatter) [4], antimatter plasmas [5], production of molecular positronium [6] and many others.

From the fundamental point of view positrons are interesting since the details of antimatter–matter interactions are still not completely understood. Among many important differences between electron and positron interactions with matter the following are particularly important [7]. First, the absence of the resonances for positrons leaves a very small non-resonant vibrational excitation [8,9]. Second, the absence of the exchange interactions leads to a smaller number of electronic states that can be excited by positron impact. Finally, the Ps formation channel, a non-conservative process unique to positrons, often has a significant cross section [10,11].

One of the main goals of positron physics today is determination of accurate cross sections for positron scattering on many different targets, both experimentally and theoretically. Recently, much effort has been invested in material studies using positron beams [12]. Although it is not in the primary focus of the scientific community, there is an increasing need for positron transport studies. The first reason is fundamental: new accurate cross sections open a possibility to apply well developed electron transport theory to positrons and to learn more about positron kinetics. A huge cross section for Ps formation, a non-conservative process unique to positrons, strongly affects positron transport inducing new interesting kinetic phenomena [13–16]. In addition to fundamental issues, the knowledge of positron transport is essential for modeling of positron traps [17] and for biomedical applications [2].

In this paper we present transport properties for positrons in H_2 under the influence of electric field. The emphasis is placed upon the effects of non-conservative nature of Ps formation on the drift and diffusion. In our previous paper [16] the applicability of the well established conditions for NDC for electron swarms was tested and new criteria for positrons were identified. This work

* Corresponding author. Tel.: +381 11 3713 157; fax: +381 11 3162 190.
E-mail address: ana.bankovic@gmail.com (A. Banković).

0168-583X/$ - see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.nimb.2011.10.060

can be seen as an extension of [16] for positron swarm in H_2. In order to get better insight into the nature of NDC phenomenon in the bulk drift velocity and also to understand the existence of a huge difference between the flux and bulk components of drift velocity and longitudinal diffusion coefficient, the spatially resolved properties of the swarm have been sampled. The well tested Monte Carlo simulation code [13,14] is used together with the multi term theory for solving the Boltzmann equation [18]. The agreement between results obtained with these two essentially different techniques is excellent but for the reason of clarity, both sets of results are not shown in all figures.

2. Results and discussion

In calculations of transport coefficients it is important to have a complete set of cross sections in order to ensure energy, momentum and particle balance in the swarm. In Fig. 1 the compilation of the best experimental [8,9,19] and theoretical [20–22] cross sections for positrons in hydrogen available from the literature is given. The energy dependence of all cross sections is reflected in the E/n_0 profiles of various transport properties shown below.

2.1. Drift velocity, NDC and diffusion coefficients

In Fig. 2 the drift velocity of positron swarm in H_2 is shown as a function of reduced electric field, E/n_0. We observe a huge difference between the flux and bulk drift velocity components. The flux drift velocity is the average velocity of all particles in the swarm, while the bulk drift velocity represents the velocity of the center of the mass of the swarm and quantitative differences between the two is a result of the explicit action of non-conservative collisions. More interesting is the qualitative difference: while the flux drift velocity is an increasing function of E/n_0 in the whole range of electric fields considered, the bulk drift velocity shows very pronounced negative differential conductivity (NDC). NDC is a kinetic phenomenon which represents the decrease of the drift speed with increasing driving field and it has been systematically investigated and explained for electron swarms during the last three decades [23–26]. In brief, NDC for electrons arise from a certain combination of inelastic–elastic cross sections and is present both in flux and bulk drift velocity [26]. For positrons, there is however no sign of NDC in the flux drift velocity component and the huge difference between flux and bulk components has never been observed for electrons. In our previous study of positron transport in argon [13,14] it is shown that the NDC effect for positrons originates from the non-conservative nature of

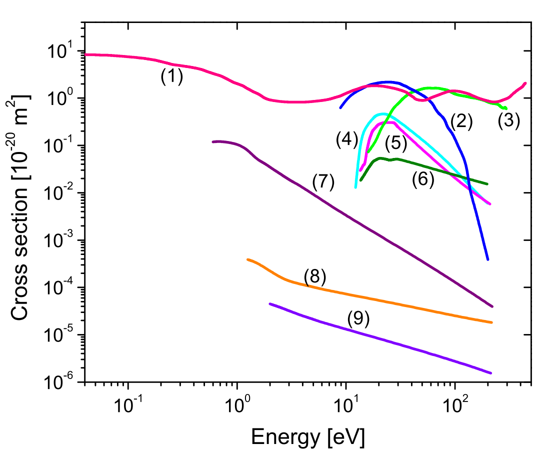

Fig. 1. Complete cross section set for positrons in H_2: (1) elastic = total [22] – all the others, (2) Ps formation [19], (3) ionization [19], electronic excitations: (4) B1Σ [9], (5) X-C [20], (6) X-E [20]; vibrational excitations: (7) v1 [8], (8) 02 [21] and (9) 03 [21].

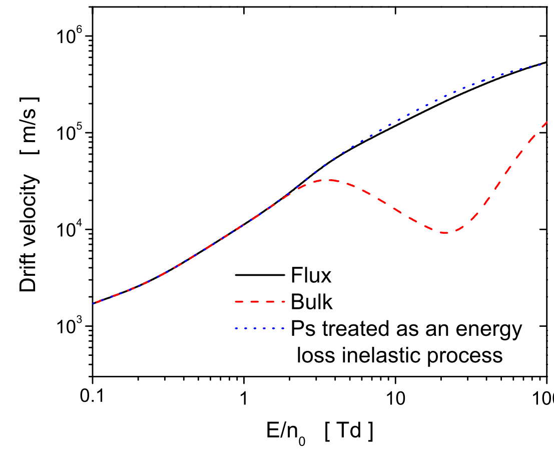

Fig. 2. Variation of the flux and bulk components of the drift velocity with E/n_0 when Ps formation is treated regularly and as an inelastic conservative process.

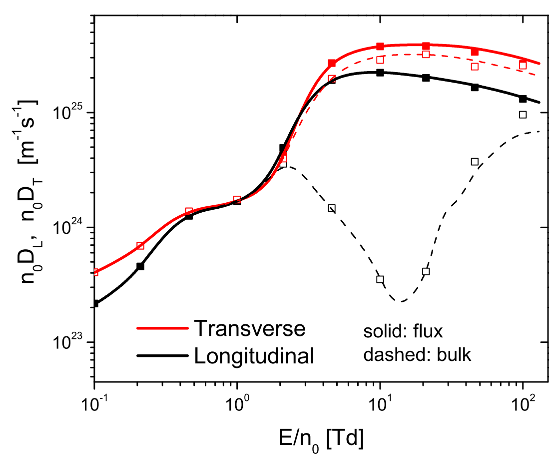

Fig. 3. Variation of the diffusion coefficients with E/n_0 for positrons in H_2.

Ps formation. When Ps formation was treated as a conservative inelastic process, the difference between two components was removed along with the NDC effect. We apply the same procedure for positrons in H_2 and results are shown in Fig. 2 (blue curve).[1] It is obvious that the significant differences between the flux and bulk components has disappeared. A small difference between the black and blue curves indicates the explicit influence of Ps formation on the velocity distribution function of positrons.

In Fig. 3 we display the flux and bulk components of the longitudinal and transverse diffusion coefficients as a function of E/n_0. The differences between the longitudinal and transverse diffusion coefficients is evidence of the anisotropic nature of diffusion which follows from the interplay of energy dependent collision frequency and spatial variation of average energy along the swarm. On the other hand, deviations of almost two orders of magnitude between the flux and bulk longitudinal diffusion components is another dramatic manifestation of the explicit non-conservative effects of the Ps formation processes.

2.2. The gradient energy vector

What is happening inside the swarm under the action of non-conservative collisions? For electron swarms, the spatial variation

[1] For interpretation of the references to color in Fig. 2, the reader is referred to the web version of this article.

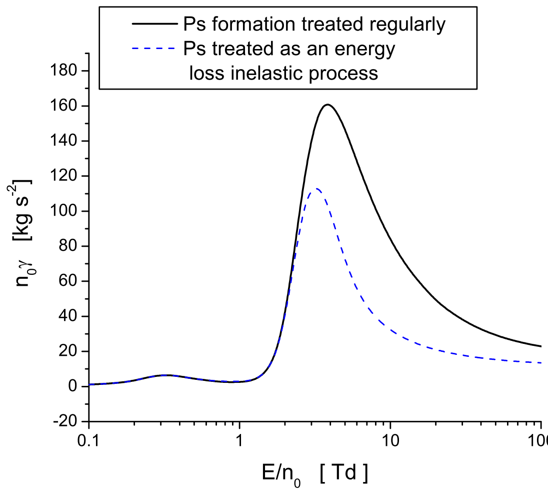

Fig. 4. Variation of the gradient energy vector with E/n_0 when Ps formation is treated regularly and as an inelastic conservative process.

of the average energy along the swarm has played a central role in the explanation of many phenomena including those associated with the implicit and explicit effects of non-conservative collisions and the anisotropic nature of the diffusion [18]. In this paper we apply the same strategy for positrons. In Fig. 4 the gradient energy vector γ is shown as a function of E/n_0: the black curve[2] corresponds to the case when Ps formation is treated regularly, as a non-conservative process, and the blue one represents the situation when Ps formation is treated as an energy loss inelastic process. The gradient energy vector represents the first order spatial variation of the average energy along the swarm, or in the language of Monte Carlo simulations, the slope of the average energy along the swarm.

For E/n_0 values lower than 2 Td there is no difference between black and blue curves, which is consistent with the trends observed in the profiles of the flux and bulk drift velocities (see Fig. 2). Between 0.1 and 0.3 Td γ is an increasing function of E/n_0. The elastic cross section is a decreasing function of energy, positrons are accelerated along the direction of the field, the average energy of the swarm is increasing and, as expected, the slope of the average energy γ is increased. In the region between 0.3 and 1 Td, the cross sections for vibration excitations start to rise, higher energy positrons at the front of the swarm are preferentially losing their energy through these collisions, and the slope of the average energy starts to decrease. From 1 to 4 Td, the cross sections for vibrational excitations have a sharp drop, positrons are accelerated again and γ has a sharp rise. The blue and black curve are identical up to $E/n_0 = 2$ Td, when the positron swarm becomes affected by Ps formation.

If Ps formation is treated as a conservative inelastic process (blue curve in Fig. 4) positrons are not lost from the swarm after 'Ps formation'. They simply lose their energy and the number of low-energy particles is locally increased, reducing spatial variation of the average energy. The sudden drop of the blue curve as a result of treating Ps formation as conservative inelastic process then follows with 'the conservative γ' peaking when Ps formation starts to dominate other processes. This trend continues with increasing E/n_0 until other inelastic channels start to affect the swarm. From that point, the slope of the average energy through the swarm decreases even more.

For E/n_0 of 2 Td the effects of the non-conservative nature of Ps formation on γ become evident. Ps formation removes the majority of positrons with the highest energies and has no influence on low-energy particles. Therefore the black curve in Fig. 4 corresponds to behavior of the remaining 'low-energy' positrons only. These positrons are accelerated by the field and the slope of the average energy is increased. Locally, at the front of the swarm, for certain fields, the number of positrons which take place in Ps formation exceeds the number of positrons that are coming from the trailing edge of the swarm accelerated by the field. As a consequence the center of the mass of the swarm is shifted opposite to the field direction which in turn induces NDC effect.

2.3. Spatial profiles of positron swarm

In Fig. 5(a) the spatial profile and spatially resolved average energy of the swarm for three distinct values of E/n_0 are shown. For $E/n_0 = 1$ Td, the energy of all particles in the swarm is well below the threshold for Ps formation (in Fig. 2 the flux and bulk components of the drift velocity are identical). For $E/n_0 = 2.1$ Td, the bulk drift velocity starts to decrease and for $E/n_0 = 10$ Td, the swarm is in the middle of the NDC region. Consequently it is interesting to understand the spatial profile of the swarms in these different situations. In order to determine the spatially resolved data, we have restricted the space and divided it into boxes. Every box contains 100 points and these points are used to sample spatial parameters of positron swarm.

For $E/n_0 = 1$ Td, the spatial profile is almost symmetric, it has a Gaussian profile and the spatial variation of the average energy is almost negligible. Small local peaks can be seen on the top of the

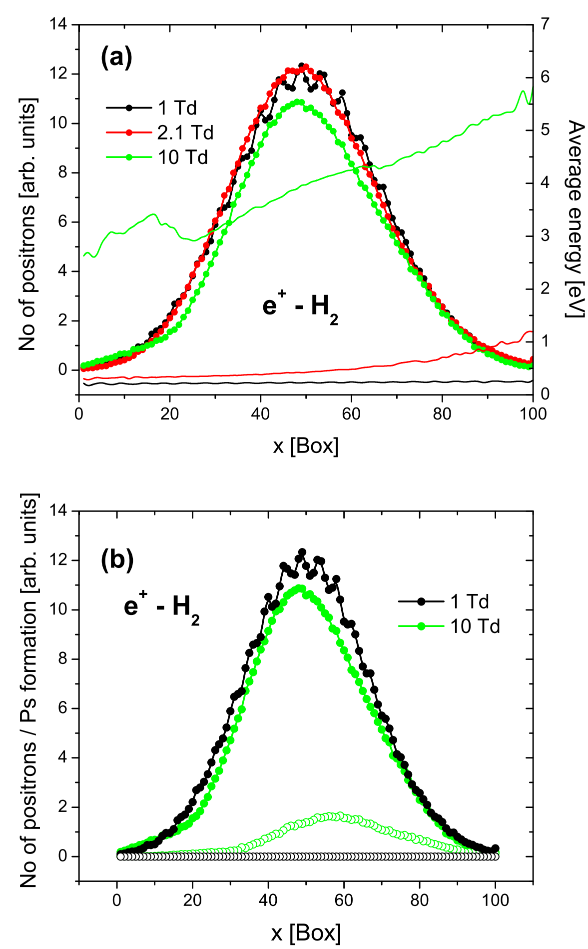

Fig. 5. (a) Spatial profile of the swarm and spatially resolved average energy for E/n_0 of 1, 2.1 and 10 Td; (b) comparison of the spatially resolved number of positrons in the swarm and number of Ps formation events for E/n_0 of 1 and 10 Td.

[2] For interpretation of the references to color in Fig. 4, the reader is referred to the web version of this article.

profile of the swarm. This is a transient phenomenon, resulting from the fact that the vibrational excitation threshold is close to the average energy of the swarm. The fastest positrons have enough energy to excite H_2 molecules, but after the collision they are pushed back to the lower energy region of the swarm. The field accelerates these positrons, so they are again able to excite H_2 molecules. The nature of these transient spatial structures is similar to those found in Franck Hertz experiment [27].

For E/n_0 of 2.1 Td, the oscillatory structure is no longer present, the profile is smoother and slightly shifted to the left. The spatial variation in the positrons average energy is now much stronger. At this energy Ps formation channel begins to open and some of the fastest positrons are removed from the swarm. For E/n_0 of 10 Td, when NDC is very pronounced, the profile of the swarm is dramatically skewed and the front of the swarm is cut off.

In order to better understand the impact of Ps formation, the spatial variation of the Ps formation events is sampled. In Fig. 5(b) the results are shown for $E/n_0 = 1$ Td and 10 Td (open symbols), together with spatial profiles of the swarm (full symbols). For $E/n_0 = 1$ Td, the number of Ps formation is zero throughout the swarm, which is expected since the average energy of the swarm is far from the threshold for Ps formation. For E/n_0 of 10 Td, spatially resolved number of Ps formation has a profile similar to the shape of the swarm and maximum of this profile is shifted to the leading edge of the swarm. Due to the spatial variation of the average energy through the swarm, Ps formation becomes a spatially selective process, giving rise to the NDC effect exists in bulk drift velocity component only and huge differences between the flux and bulk components of the longitudinal diffusion coefficients.

3. Conclusion

In this work the influence of non-conservative collisions on positron transport is analyzed by sampling the spatially resolved properties of the swarm. Calculated transport properties including gradient energy vector, spatial profiles of the swarm and spatially resolved average energy and Ps formation profiles have given a new insight into (i) NDC phenomenon and (ii) the explicit effect of Ps formation on the diffusion tensor elements. The extremely skewed spatial density profiles of positron swarms suggest that it would be important to calculate high-order transport coefficients. Such information can help in the design of future positron experiments as well as in the interpretation of their results.

Acknowledgments

This work was supported by MNRS Project ON171037 and III41011 and Australian Research Council. S.D. acknowledges also support from STW-project 10118, part of the Netherlands' Organization for Scientific Research (NWO).

References

[1] N. Guessoum, R. Ramaty, R.E. Lingenfelter, Astrophys. J. 378 (1991) 170.
[2] G. Muehllehner, J.S. Karp, Phys. Med. Biol. 51 (2006) R117.
[3] L.D. Hulett Jr., D.L. Donohue, J. Xu, T.A. Lewis, S.A. McLuckey, G.L. Glish, Chem. Phys. Lett. 216 (1993) 236.
[4] M. Amoretti et al., Nature 419 (2002) 456.
[5] C.M. Surko, R.G. Greaves, Phys. Plasmas 11 (2004) 2333.
[6] D.B. Cassidy, S.H.M. Deng, R.G. Greaves, T. Maruo, N. Nishiyama, J.B. Snyder, H.K.M. Tanaka, A.P. Mills Jr., Phys. Rev. Lett. 95 (2005) 195006.
[7] M. Charlton, J. Humberston, Positron Physics, Cambridge University Press, New York, 2000.
[8] J.P. Sullivan, S.J. Gilbert, C.M. Surko, Phys. Rev. Lett. 86 (2001) 1494.
[9] J.P. Sullivan, J.P. Marler, S.J. Gilbert, S.J. Buckman, C.M. Surko, Phys. Rev. Lett. 87 (2001) 073201.
[10] J.P. Marler, J.P. Sullivan, C.M. Surko, Phys. Rev. A 71 (2005) 022701.
[11] G. Laricchia, P.V. Reeth, M. Sluzinśka, J. Moxom, J. Phys. B: At. Mol. Opt. Phys. 35 (2002) 2525.
[12] J.P. Sullivan, J. Roberts, R.W. Weed, M.R. Went, D.S. Newman, S.J. Buckman, Meas. Sci. Technol. 21 (2010) 085702.
[13] M. šuvakov, Z.Lj. Petrović, J.P. Marler, S.J. Buckman, R.E. Robson, G. Malović, New J. Phys. 10 (2008) 053034.
[14] J.P. Marler, Z.Lj. Petrović, A. Banković, S. Dujko, M. šuvakov, G. Malović, S.J. Buckman, Phys. Plasmas 16 (2009) 057101.
[15] A. Banković, J.P. Marler, M. Šuvakov, G. Malović, Z.Lj. Petrović, NIMB 266 (2008) 462.
[16] A. Banković, Z.Lj. Petrović, R.E. Robson, J.P. Marler, S. Dujko, G. Malović, NIMB 267 (2009) 350.
[17] S.J. Gilbert, C. Kurz, R.G. Greaves, C.M. Surko, Appl. Phys. Lett. 70 (1997) 1944.
[18] S. Dujko, Z.Lj. Petrović, R.E. Robson, Phys. Rev. E 81 (2010) 046403.
[19] D. Fromme, G. Kruse, W. Raith, G. Sinapius, J. Phys. B: At. Mol. Opt. Phys. 21 (1988) L261.
[20] F. Arretche, M.A.P. Lima, Phys. Rev. A 74 (2006) 042713.
[21] F.A. Gianturco, T. Mukherjee, Phys. Rev. A 64 (2001) 024703.
[22] K.R. Hoffman, M.S. Dababneh, Y.F. Hsieh, W.E. Kauppila, V. Pol, J.H. Smart, T.S. Stein, Phys. Rev. A 25 (1982) 1393.
[23] Z.Lj. Petrović, R.W. Crompton, G.N. Haddad, Aust. J. Phys. 37 (1984) 23.
[24] Z.Lj. Petrović, Ph.D. Thesis, Australian National University, 1985.
[25] R.E. Robson, Aust. J. Phys. 37 (1984) 35.
[26] S.B. Vrhovac, Z.Lj. Petrović, Phys. Rev. E 53 (1996) 4012.
[27] R.E. Robson, B. Li, R.D. White, J. Phys. B: At. Mol. Opt. Phys. 33 (2000) 507.