RELAXATION OF LOW ENERGY
POSITRONS IN MOLECULAR GASES

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Abstract. The calculations of thermalization times and spatial relaxation profiles of the positron transport properties in H_2, N_2 and in mixture of N_2 and CF_4 are presented. Recently, the data needed to compile comprehensive set of cross sections for these gases became available which made our calculations possible. The main difference between positron and electron transport is the existence of the effect of positronium (Ps) formation which changes the number of particles and has a strong energy dependence. The relative magnitude of positronium formation to electronic excitations and the relative positions of their thresholds control the efficiency of thermalization and non-conservative transport phenomena. The effect of vibrational and rotational excitations on thermalization has been considered and relative contributions were determined. Our calculated thermalization data are in reasonably good agreement with the experimental data of Al-Qaradawi et al. (2000).

1. INTRODUCTION

The investigation of low energy positron interactions with matter is of great interest in areas of atomic physics, condensed matter physics and gamma-ray astronomy. There is also a need to understand these interactions for technological applications including mass spectroscopy, characterization of solid surfaces and for biomedical diagnostics. Progress in positron-matter interaction research has been limited by the availability of high flux positron sources and bright low-energy positron beams. The development of efficient positron traps (e.g. the Penning-Malmberg-Surko trap) changed this situation.

The development of low energy positron traps opened a possibility of measuring the low energy cross sections for positron scattering on numerous gases and allowed us to revisit the studies of positron transport and possible interpretations of past and future swarm experiments. We have compiled reasonably complete sets of cross sections for several gases such as nitrogen, hydrogen, water vapor and argon (see Šuvakov et al. (2008) and Banković et al. (2008)) and performed calculations of transport coefficients.
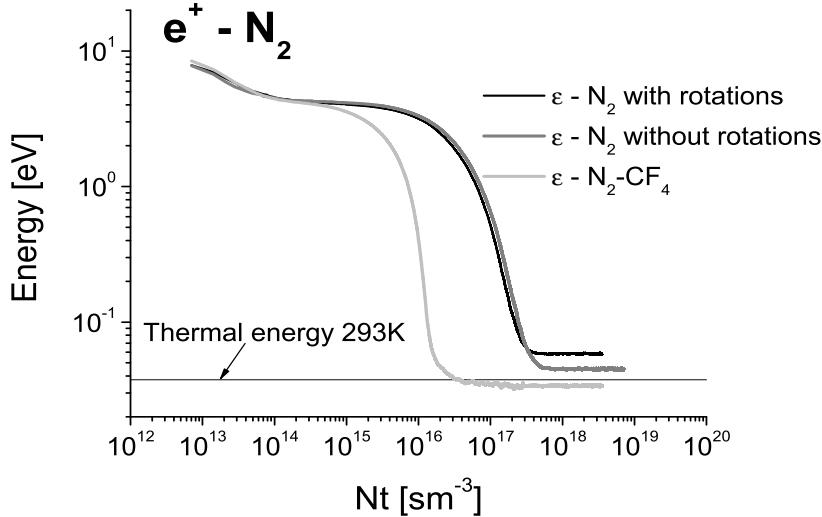
Figure 1: Thermalization of the mean energy of positrons from a Maxwellian initial distribution with a mean starting energy of 10 eV in N_2 and N_2-CF_4 mixture.

2. TEMPORAL RELAXATION

We have performed Monte Carlo simulation of thermalization for the energy range relevant to the Penning-Malmberg-Surko trap at the room temperature (293 K). The main goal of this work was to give the estimate of thermalization times for positrons in different gases and perhaps to open a possibility to optimize gas composition and performance of these traps. Thermalization time has been defined as the time it takes positrons to reach the energy 50% above the thermal equilibrium energy in gases but for practical purposes we took it to mean the time it takes to reach twice the thermal energy. The results have been compared with experimental measurements of Al-Qaradawi et al. 2000. who used the positron lifetime spectroscopy in order to obtain the thermalization times. When making comparisons such as this, one should bear in mind that it is very difficult to provide identical definition of the boundary for thermalization when time is determined in two approaches.

Temporal relaxation of positrons from Maxwellian with the mean starting energy of 10 eV in nitrogen is presented in Figure 1. In the same Figure, it is shown how rotational excitations affect the thermalization of positrons. The rotational excitations are quite small in nitrogen and they make little contribution even below 100 meV. Here we have assumed that the cross sections for rotational excitation are the same as for non-resonant rotational excitation by electrons. Addition of other molecular gases such as CF_4 with large vibrational cross sections speeds up thermalization while the overall losses to Ps formation are not increased significantly. In Figure 1 the thermalization in mixture of N_2 with 10% of CF_4 is presented. We observe that the time of thermalization becomes shorter by an order of magnitude when CF_4 is added to the molecular nitrogen.
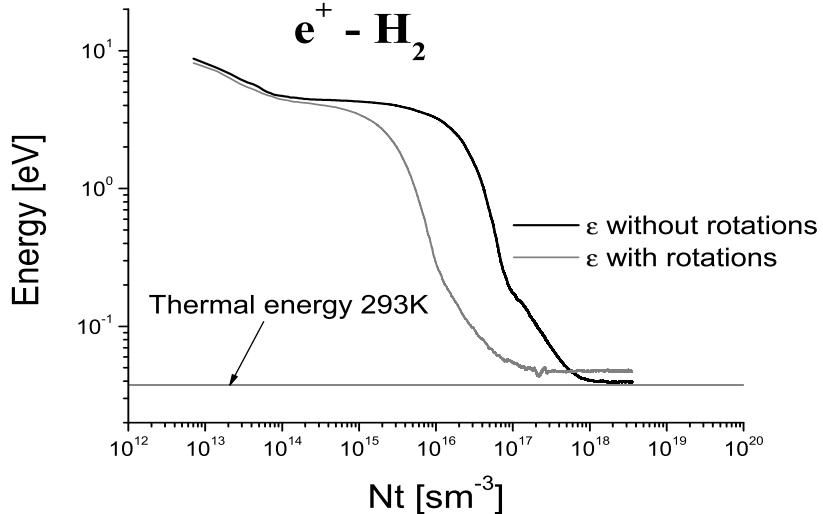
Figure 2: Thermalization of the mean energy of positrons from a Maxwellian initial distribution with a mean starting energy of 10 eV in H_2.

In Figure 2 the similar results for positrons in hydrogen are presented. The rotational excitations in hydrogen are much larger then those in nitrogen so their influence on the thermalization time is significantly larger and it becomes essential for thermalization to energies below 100 meV, making hydrogen almost as effective in thermalization as the mixture of N_2 and CF_4. The main reason why it is more convenient to use molecular nitrogen as buffer gas in positron traps than molecular hydrogen is the relative position of the threshold for Ps formation to electronic excitations threshold. In H_2 the threshold for Ps formation is lower than the thresholds for electronic excitations and thereby losses of positrons during thermalization will be far greater as compared to nitrogen.

The thermalization time has been extracted from Figures 1 and 2. The moment when positrons are in thermal equilibrium with surrounding gas has been defined as the time that positron need to reach the half of the thermal energy above $3kT/2$. Thermalization times measured by Al-Qaradawi et al. 2000. have been given originally in units of ns Amagat (1 Amagat $= 2.69 \times 10^{25}$ sm^{-3}) and here these units are converted to sm^{-3}. The comparison between our Monte Carlo calculations and experimental results is presented in Table 1. One should bear in mind that in experiment the limiting time is determined by the energy resolution of the experiment. Our choice of the energy 50% above the thermal energy is rather arbitrary but it was selected to reduce uncertainties in determination where the slope of the curve is still high. The experimental data are in good agreement with our data but are more consistent with resolution of the order of 20% above the thermal energy. In any case we may state that our results are in good agreement with the experiment.

When considering comparisons with the thermalization times in Surko trap one should redefine the calculation to use initial distribution (of velocities) that is more appropriate to the trap.

Table 1: Comparison between the thermalization times calculated using our Monte Carlo code and measured by Al-Qaradawi et al. 2000

gas	Nt (sm^{-3}) Present results	Nt (sm^{-3}) Al-Qaradawi et al
N$_2$	2.5×10^{17}	3.8×10^{17}
N$_2$-CF$_4$	1.4×10^{16}	X
H$_2$	4.5×10^{16}	6.5×10^{16}

3. SPATIAL RELAXATION

A standard Surko trap belongs to Steady state Townsend (SST) experiments in strongly non-hydrodynamic conditions, i.e. with very few collisions bordering on beam experiments. We have treated spatial relaxation of the initial distribution paying special attention to the mean energies and average velocities. The data were obtained by our steady-state Townsend (SST) Monte Carlo simulation code. Both the mean energy and average velocity exhibit a damped oscillatory relaxation along a decaying profile for $E/N > 0.25$ Td. The nature of the spatial relaxation profiles of positron transport properties is dependent as the interplay between the power dissipated in elastic collisional processes, power dissipated in inelastic collisions and power deposited into the swarm by the field. For certain gases there exist a window of E/N strengths where the relaxation profiles are damped oscillatory in nature, and outside this window the profiles are monotonic.

4. CONCLUSION

In our attempt to apply modern tools for a treatment of the electron swarms to positron transport, we have performed calculations for thermalization of positrons at sub excitation (less than 10 eV) energies. Our calculated results provide a tool for optimizing the collisional traps and thermalization/annihilation experiments. The calculated thermalization times are in good agreement with experimental data giving support to the selected set of cross sections as the numerical technique has been verified independently.

References

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