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DIFFUSION COEFFICIENTS OF H_2^+ IONS IN H_2 GAS

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Abstract. In this work we present a complete cross sections set and transport properties of H_2^+ in H_2 gas. Ionic charge transfer reactions with molecules are indispensable elementary processes in the modeling of kinetics in terrestrial, industrial and astrophysical plasma in the detection of dark matter. A Monte Carlo simulation method is applied to accurately calculate transport parameters in hydrodynamic regime. We discuss new data for H_2^+ ions in H_2 gas where the mean energy, longitudinal and transversal diffusion coefficients are given as a function of low and moderate reduced electric fields *E/N* (*E*-electric field, *N*-gas density).

1. INTRODUCTION

Transport properties of species in gas plasmas are of great importance in understanding the nature of molecular and ionic interactions in gas mixtures (Todd et al. 2002, Mason 1957, Golzar et al. 2014). These properties include the mean energy, drift velocity, diffusion coefficients, ionization and chemical reaction coefficients, chemical reaction coefficients for ions and (rarely) excitation coefficients, and they are very useful in chemical industries for the design of many types of transport and process equipment.

We notice the importance of obtained results as atomic and molecular data which are input parameters for modeling of various environments. Low temperature can change the state of metals, gases, liquids and solids, cause damage to organisms depending on length of exposure, and change the functionality of mechanized processes. Quantum-mechanical calculation of a certain cross-section is a required task that requires knowledge of the surface potential energy of ions and molecules to be constructed from the structure of the reactants. Less intensive computational methods, such as the Denpoh-Nanbu theory (Denpoh and Nanbu 1998, Nikitović et al. 2014, Petrović et al. 2007), require knowledge of thermodynamic formation data and are applicable to a range of molecules.

2. CROSS SECTION SETS

Ion charge transfer reactions with molecules are important elementary processes in modeling kinetics in all types of plasma. In many cases, it is known

that the cross section for these reactions represents the most important part of the set of cross section. Transport properties needed for modeling H_2 discharges containing H_2^+ ions are calculated by the Monte Carlo method. A code that properly takes into account thermal collisions was used (Ristivojević and Petrović 2012). The cross-section set describes the total collision cross-section between an ion and a gas particle. The total collision cross-section between an ion and a gas particle is described at low energies using Langevin's cross-section and at higher energies using the collision of rigid spheres, as demonstrated in paper (Nikitović et al. 2016, Nikitović et al. 2019).

Figure 1 presents a complete set of cross sections for ion-H_2 molecule interactions as a function of collision energy. The provided cross sections by (Denpoh and Nanbu, 2022) are presented, except for those for proton transfer, H^+ production, and charge exchange, for which the cross sections were obtained from Phelps' work (Phelps 1990, Phelps 2011). The set encompasses rotational (H_2^+ + H_2, Rot.), vibrational (H_2^+ + H_2, Vib.), electronic (H_2^+ + H_2, El. ex.), and dissociative (H_2^+ + 2H, Diss. ex.) excitations, in addition to Neutral dissociation (H_2^+ + 2H, Neutral dissociation) and Ionization (H_2^+ + H_2^+ + e, Ionization), as well as dissociative ionization (H_2^+ + H^+ + H + e, Diss. Ionization) along with the other mentioned processes. The reaction products of H_2^+ + H_2 shown in parentheses, along with the corresponding labels on the Figure 1.

Non-elastic excitation processes are treated isotropically. In the case of ionization processes, the secondary ion H_2^+ is also tracked, which shares the incoming kinetic energy with the primary ion reduced by the reaction threshold. The partition of kinetic energy between the primary and secondary ions is determined randomly. In the case of proton transfer processes, the resulting ion H_3^+ is not tracked in the simulations, nor is the H^+ ion in the case of H^+ production.

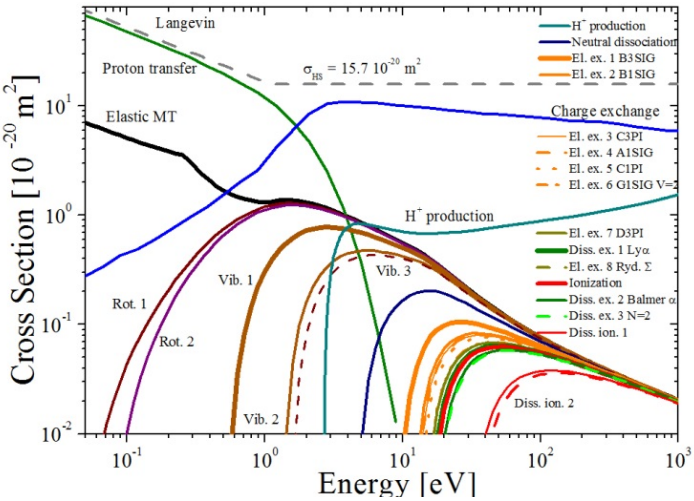

Figure 1: Complete set of cross sections for ion (H_2^+) and molecule (H_2) interactions as a function of collision energy.

2. RESULTS AND DISCUSSION

Proton transfer reactions deplete the swarm of low-energy H_2^+ ions, resulting in a mean ion energy of 0.37 eV at E/N = 1 Td, which is significantly higher than the thermal energy of H_2 molecules at T =300 K in Figure 2. The rise in mean energy is strongly resisted by charge exchange, rotational and vibrational excitation as the electric field increases. With increasing energy, the rate of charge exchange reactions decreases, allowing the mean energy to rise more quickly after E/N > 200 Td.

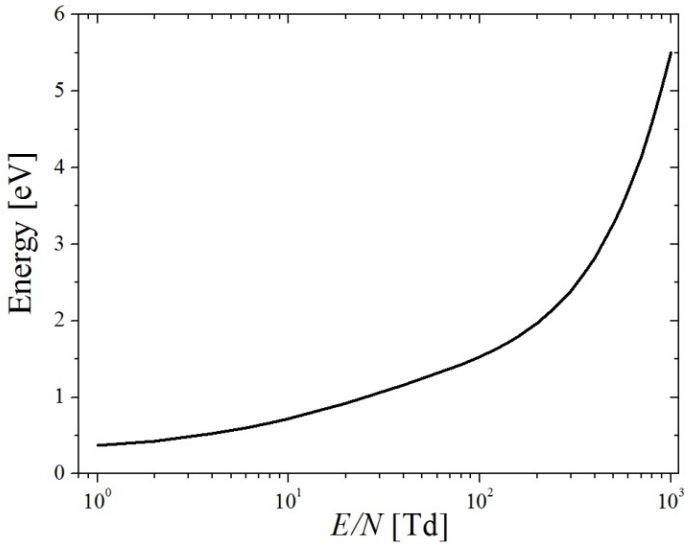

Figure 2: Mean energy of H_2^+ ions a function of E/N at 300 K.

In Figure 3, the bulk and flux values of longitudinal and transverse diffusion coefficients, multiplied by the gas concentration, are shown as a function of E/N. For E/N < 100 Td, the significantly lower D_L than D_T indicates highly anisotropic diffusion of the swarm, which spreads four times slower in the direction of the field, deforming the swarm's spherical shape into a highly ellipsoidal shape.

The reduction of diffusion coefficients with increasing E/N is attributed to the rising number of charge exchange reactions with energy that produce slow H_2^+ ions. While there are minor differences between the bulk and flux values of diffusion coefficients, as evident in Figure 3, except for transverse diffusion at low fields, where the bulk values surpass the flux values.

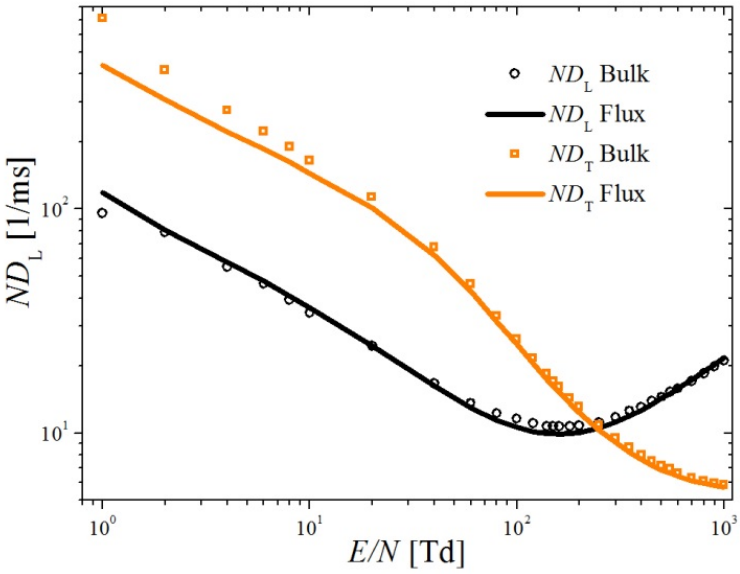

Figure 3: Bulk and flux longitudinal and transverse diffusion coefficients as a function of *E/N* at 300K.

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