Collision-radiative model for study of electron temperature in cryogenic afterglow plasma

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Abstract: Our afterglow study of recombination of H_3^+ ion in conditions relevant to insterstellar medium (ISM) initiated the development of a computer model that is able to determine the electron temperature for data interpretation. From the model of chemical kinetics in afterglow plasma it follows that there is a connection between electron temperature and vibrational state population of molecular hydrogen. For better results and our understanding, a collision-radiative model is being developed now.

Keywords: Chemical kinetics, low temperature plasma, collision-radiative model.

1. Introduction

Due to the amount of hydrogen in the interstellar space it is important to understand its behavior at low temperature. For that purpose its elementary reactions are being studied in conditions relevant to the ISM. The H_3^+ ion plays an important role in this environment as it initiates many complex reactions. [1]

For a deeper understanding of processes in the ISM and for astrophysical models, it is important to understand the destruction of the H_3^+ ion. Recombination in the afterglow plasma is studied for this purpose in our group. [2,3]

The measurments are performed with Stationary Afterglow – Cavity Ring Down Spectrometer aparature at temperatures of the neutral partical and ions between 40 and 300 K. Rate coefficient of recombination is determined from the decay of the ion number density in the afterglow. The number density is obtained from the absorption spectra. The experiments are carried out in a mixture of helium and hydrogen with argon admixture. The current form of the aparature does not allow measurment of electron temperature which can be crucial for the studied processes. For better interpretation of measured data it is important to create a computer model which can determine the electron temperature. The model will also be used for design of new experiments.

2. Model of chemical kinetics

The first created model contains a balance equation for electron temperature including the influence of collisions with rotationaly excited H_3^+, Coulomb collisions, elastic collisions with helium and elastic, inelastic and super-elastic collisions with molecular hydrogen. The obtained results show the possibility of interconnection of electron temperature and population of vibrational states of molecular hydrogen.

More detailed chemical kinetics was applied to the model which among other things more specifically determines the population of the vibration states of molecular hydrogen.

The chemical kinetics model contains 86 reactions. Electron temperature is influenced primarily by:

- elastic collisions
- inelastic collisions
- super-elastic collisions
- Coulomb colisions

Other processes in the model are collisions between neutral particles and ions and diffusion of the particles onto the wall of the discharge tube. Interaction with the wall is an important process. For ions and electrons it leads to recombination. Atomic hydrogen can also recombine on the wall, producing vibrationally excited hydrogen molecules, which are returned to the plasma. This leads to the supply of energy to the electrons due to super-elastic collisions. On the other hand, diffusion of the excited molecules also leads to deexcitation on the wall.

Technically, electron temperature is included in the chemical kinetics model as a “species” that has its own ordinary differential equation. Terms of the equation are contributions from the relevant processes.

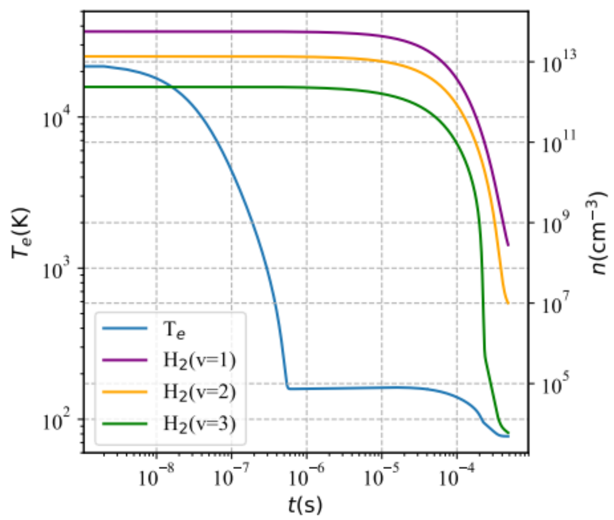

Fig. 1. Time evolution of vibrational states of H2 and electron temperature in the afterglow. Conditions are mentioned in the results section.

3. Results

The model was applied at a pressure of 1000 Pa, neutral temperature of 77 K and electron temperature of

22700 K. The initial concentration of helium was [He] = 9.41 10^{17} cm^{-3}. Concentrations of argon and molecular hydrogen were [Ar] = [H_2] = [He] / 1000 cm^{-3}.

Firstly, the model calculated concentrations of all species in the discharge. It stopped after reaching equilibrium. After that, the model started counting electron cooling.

The result of the chemical kinetics model confirms the interconnection between electron temperature and population of vibrational levels of molecular hydrogen. This result is shown in Fig. 1. In the table 1, there are compared processes which play a role in an evolution of electron temperature for better understanding. Contributions are taken relative to cooling by elastic collisions. Thus, a positive sign indicates cooling and negative heating of electrons.

Table 1: Realive influence of interaction on an evolution of electron temperature

Time [s]	Elastic	Inelastic	Super-Elastic	Coulombic
0	1	0.040	-0.004	0.002
$1\cdot10^{-7}$	1	0.039	-0.013	0.028
$1.5\cdot10^{-7}$	1	0.014	-0.011	0.066
$4.2\cdot10^{-7}$	1	$8.6\cdot10^{-10}$	-0.008	1.441
$1\cdot10^{-6}$	1	$1.5\cdot10^{-24}$	-9.472	8.467
$1\cdot10^{-5}$	1	$2.1\cdot10^{-24}$	-5.933	4.933
$5\cdot10^{-5}$	1	$8.3\cdot10^{-26}$	-2.912	1.914
$1\cdot10^{-4}$	1	$1.3\cdot10^{-28}$	-2.238	1.241
$3\cdot10^{-4}$	1	$5.3\cdot10^{-44}$	-1.945	0.961

Firstly, there is rapid cooling by elastic collisions with neutrals in the afterglow. The cooling continues until the influence of heating by super-elastic collisions is sufficient to stop losses. The influence of inelastic collisions is completely negligible by that time. The main cooling process are Coulomb collisions now. Electron temperature is held almost constant, as is the concentration of excited H_2 states. At a time corresponding to the characteristic diffusion time of H_2 (~150 μs), the population of excited particles decreases. That leads to a decrease in the effect of super-elastic collisions and so the electron temperature drops as well.

The model also suggests that at time t ~ 150 μs after turning off discharge, which almost coincides with the time when we start measuring recombination, electron temperature is T ~ 80 K. Thus, the results of the model lead to the question how large the effect of electron cooling is on the measurement of recombination and what other processes can significantly affect the electron temperature.

4. Collision-radiative model

In order to better understand the interaction of electrons with excited particles in the discharge and in the afterglow, we are now creating a collision-radiative model that could be verified by comparing the calculated spectrum with the emission spectrum measured in the experiment. The radiation will result in additional energy losses from the system, thus potenttially cooling the electrons. Fitting model parameters should also lead to better determination of the electron distribution function and thus further refine the model results.

5. References

[1] T. Oka, Chemical Reviews, **113**, 8738 (2013).
[2] R. Plašil et al., Review of Scientific Instruments, **89**, 063116 (2018).
[3] P. Dohnal et al., Physical Chemistry Chemical Physics, American Physical Society, **18,** 34 (2016).