Available online at www.sciencedirect.com
ScienceDirect
Radiation Physics and Chemistry 76 (2007) 573–576
Radiation Physics and Chemistry
www.elsevier.com/locate/radphyschem

Vibrational excitation coefficients for electrons in HBr

Olivera Šašić, Zoran Lj. Petrović*

Institute of Physics, POB 68, 11080 Belgrade, Serbia and Montenegro

Received 31 August 2005; accepted 20 September 2005

Abstract

Rate coefficients were calculated for the first time for vibrational excitation in pure HBr in both DC and RF, E and in ExB fields. We have studied the effect of the amplitude and frequency of applied fields. The calculation was based on a Monte Carlo technique. It was found that a complex behavior may develop due to sharp and very large vibrational cross sections and modulation of the energy distribution function by time-dependent fields and by magnetic field.

Keywords: Rate coefficient; Vibrational excitation; Monte Carlo; HBr; Time-dependent fields; Crossed fields

1. Introduction

In recent years, we have seen an extensive use of low-pressure plasmas in hydrogen halide containing gases in various applications such as electron pumped lasers, plasma etching technologies and fabrication of optoelectronic devices (Bestwick et al., 1991; Chang et al., 1996; Xu et al., 2001). Development and optimization of these applications are closely connected with better understanding of many kinetic phenomena that may occur in plasmas, and further improvements in charged particle transport theory. Many techniques have been developed in order to get more precise and detailed models of both DC and RF discharges (Nakano et al., 1994; Marić et al., 2003; Robson et al., 2005). Rate coefficients of single processes are, as well as the transport coefficients and cross sections, the necessary input data in fluid plasma modeling (Robson et al., 2005). At the same time the rates are often produced from complete sets of cross sections and for most gases used in plasma processing, there is a lack of reliable and complete sets of data. This often leads to some simplifications in the cross section sets. One of the most critical gases where until recently there was a complete shortage of cross section sets and transport data are HBr which is widely used in a number of applications (Bestwick et al., 1991; Chang et al., 1996; Xu et al., 2001).

In addition, lack of available transport data and understanding of the kinetic phenomena in electron transport leads to additional simplifications such as the extrapolation of transport data obtained for constant field to RF plasma models, through corresponding effective values. Furthermore, the effect of magnetic field usually is not taken into account. The present paper attempts to remedy the shortage of transport data for HBr by presenting rate coefficients for vibrational excitation for different conditions including the RF fields and the effect of magnetic fields.

In the region of low electron mean energies, which we chose to investigate, the dominant feature in the inelastic energy losses, determining the properties of electron swarms, are the vibrational excitation cross sections. That, together with recent excellent experimental and theoretical results for those cross sections, was the motivation factor for us to calculate the rate coefficients for those processes in case of electron scattering with HBr molecules.

As complete sets of cross sections for electrons in HBr have not been reported so far in the literature, we have compiled (Šašić and Petrović, 2006) a set consisting of the existing data from the literature with some necessary extrapolations that we have made. Unlike other processes, vibrational excitation cross sections of the hydrogen bromide have been the object of several theoretical and

*Corresponding author.
E-mail address: zoran@phy.bg.ac.yu (Z.L. Petrović).

0969-806X/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.radphyschem.2005.09.022

experimental studies (Rohr, 1978; Horáček and Domcke, 1996; Čižek et al., 2001). In our calculations, we used the results obtained by Čižek et al.(2001).

Due to considerable dipole moment of the HBr molecule, which is $0.307ea_0$, and a relatively large polarizability of the molecule, these cross sections have very high and sharp peaks. Their mean value is relatively high, too. The effect is more pronounced if the peak is closer to the threshold for dissociative attachment process. Namely, the threshold peaks of higher channels are wider and they are much smaller than those for the $v = 0 \rightarrow 1$ channel. In addition, some oscillatory structure can be seen in the threshold peak for the $v = 0 \rightarrow 1$ transition. Besides that, vibrational excitation cross sections dominate in the same energy region where Ramsauer–Townsend (RT) minimum in the elastic cross section occurs. This particular set of circumstances was found to be the most difficult for approximate treatments such as two-term approximation(TTA). The best recourse for electron transport treatment in HBr is thus some exact technique such as Monte Carlo (MC) simulation. In order to emphasize this fact, we made some comparisons of results obtained by MC simulation and by solving Boltzmann kinetic equation in TTA.

2. Calculation technique

Our Monte Carlo simulation code, which had been described in great details elsewhere (Bzenić et al., 1999; Petrović et al., 2002; Dujko et al., 2005), was used to calculate the vibrational excitation rate coefficients. We followed the spatiotemporal evolution of each electron through time steps in order to represent correctly the motion of electrons in external RF fields. The moment of collision was determined from integral collision probability. It should be noted that under the swarm conditions the electron density is sufficiently small that electron–electron interactions can be regarded as negligible. All electron transport properties were sampled at the end of very small time steps. The time steps were determined by the minimum of three constants: mean collisional time, cyclotron period (in case of constant crossed fields), and period of time-depended fields. After relaxation, all the transport properties results were averaged over all electrons in the simulation and over time. (In this paper results obtained for RF fields are presented over a single period of the field but averaging could be performed over several periods.) It is obvious that the number of initial electrons, which are included in the simulation, is a critical factor that greatly affects both statistic quality of the results and duration of the simulation. Our simulations were performed with 5×10^5 initial electrons. The gas number density was $3.54 \times 10^{22}\,\mathrm{m}^{-3}$, which corresponded to the pressure of 1 Torr (133.3 Pa) at the temperature of 273 K. Initial electron energy distribution was Maxwellian with the mean energy of 1 eV, and the phase between electric and magnetic fields was 90°. We should also note that all electron scattering was assumed to be isotropic. This assumption is not critical as there is averaging of a large number of electrons.

In case of a constant electric field, we have also made some calculations of vibrational excitation rate coefficients by using two-term Boltzmann equation solver ELENDIF (Morgan and Penetrante, 1990).

3. Results and discussion

In this section we show the basic results of rate coefficients for the excitation of vibrational levels in HBr from the ground state. The cross section set that we used in our calculation included data for eight levels. However, we only show the results of some of them, as the conclusions are generally applicable.

In Fig. 1, we show the dependence of vibrational excitation rate coefficients (K_{vib}) for the first four vibrational levels in HBr on reduced electric field ($1\,\mathrm{Td} = 10^{-21}\,\mathrm{V\,m^2}$). As it can be seen from the figure, K_{vib} increases with the electric field, since the electron mean energy is below the threshold and as it increases the overlap of the distribution function with the cross section increases as well. Region where K_{vib} reaches the maximum value corresponds to the energy region where the elastic cross section goes through the RT minimum and the vibrational excitation through the maximum. From that point to the right, K_{vib} decreases slightly since more and more electrons manage to gain enough energy to excite electronic states of HBr molecules (the energy threshold for the first excited electronic state is 6.56 eV). The differences between the results obtained by MC simulation and by the two-term code, are quite large due to unusually large vibrational excitation cross sections.

In Figs. 2 and 3, we show the dependencies of K_{vib} for the first two vibrational levels in HBr on reduced electric field for various values of reduced magnetic field (B/N) in case when external crossed electric and magnetic fields are applied. We made calculations for $B/N = 100$, 500, 1000

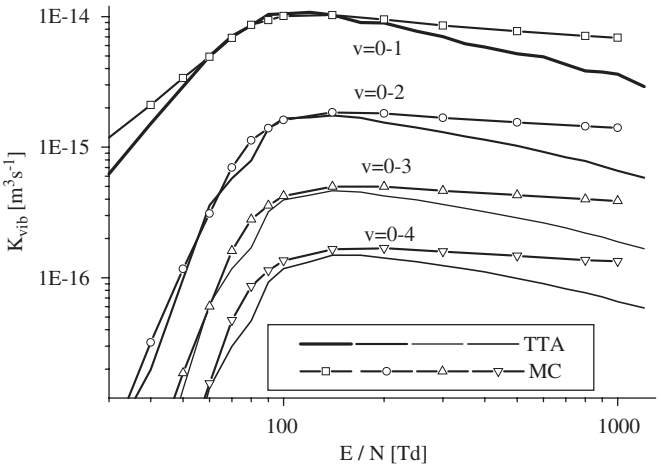

Fig. 1. Rate coefficients for excitation of: $v = 1, 2, 3, 4$ vibrational levels in HBr.