Dissociation of molecular hydrogen in a microwave discharge: kinetics of population of electronically excited states of hydrogen atoms

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Interest in the study of physico-chemical processes in microwave discharge at low and moderate pressures in hydrogen is due to the various applications of hydrogen-containing low-temperature plasma in plasma-chemical technologies. An important role in the research of hydrogen plasma is given to emission spectroscopy [1]. The molecular bands of molecules and atomic hydrogen lines they are dominated in the emission spectrum of the plasma. The internal logic of the development of plasma chemistry dictates the development of a rapid, affordable price and least time-consuming experimental - computational techniques based on combination of methods of emission spectroscopy [1] and level - to - level collisional - radiative models of atomic - molecular plasma [2]. This combination significantly expands the diagnostic capabilities of emission spectroscopy. The application of these methods allows: 1) for obtaining data on mechanisms of physical-chemical processes responsible for the formation of non-equilibrium distribution of populations of particles (molecules and hydrogen atoms, their ions) in excited radiating states; 2) for optimizing the input of reagents and catalytic additives in the discharge zone and output that of the reaction products; 3) for performing the selection of the atomic lines and molecular bands in the emission spectrum for the diagnostics of plasma parameters. Insufficient degree of completeness of the kinetic schemes (the number of quantum states and the elementary physico-chemical processes) of the formation and destruction of excited states of molecules and atoms of hydrogen of models of the atomic-molecular plasma reported in the literature limits their use for spectroscopic plasma diagnostics. In papers [3-7], it is focused on the development of molecular level – to - level models of hydrogen plasma to study the processes with participation of hydrogen molecules in the excited singlet and triplet states, which are of interest for emission spectroscopy of microwave discharge, DC glow discharge, pulsed glow discharge and plasma under conditions of electron-cyclotron resonance. This paper is devoted to the further development of the level - to - level semiempirical collisional-radiative model of molecular hydrogen plasma to investigate the processes of dissociation of molecular hydrogen and populations of electronically excited states of the hydrogen atom in microwave discharges at low and moderate pressures [7].

References

1. Ochkin V.N., Spektroskopiya nizkotemperatutrnoi plazmy (Spectroscopy of Low-Temperature Plasma), Moscow: Fizmatlit, 2006. (in Russian)
2. Biberman L.M., Vorob’ev V.S. and Yakubov I.T. Kinetika neravnovesnoi nizkotemperatutrnoi plazmy (Kinetics of Nonequilibrium Low-Temperature Plasmas), Moscow: Nauka, 1982. (in Russian)
3. Shakhatov V.A., Lebedev Yu.A., Lacoste A., Bechu S. High Temperature. 2015. Vol.53. №4. P.569.
4. Shakhatov V.A., Lebedev Yu.A., Lacoste A., Bechu S. High Temperature. 2016. Vol.54. №1. P.123.
5. Shakhatov V.A., Lebedev Yu.A., Lacoste A., Bechu S. High Temperature. 2016. Vol.54. №4. P.467.
6. Shakhatov V.A., Lebedev Yu.A., Plasma Physics Report. 2017. Т.43. №10. P.1016.
7. Shakhatov V.A., Lebedev Yu.A. High Temperature. 2017. V.55. Issue 4. P.496.