KINETICS OF PROCESSES IN the MICROWAVE DISCHARGE IN LIQUID *n*-HEPTANE includING THE SOLID PHASE

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Nonequilibrium discharges in various liquids are the subject of intensive research in recent decades [1,2]. The use of the microwave discharge as a plasma system is an effective means of carrying out plasma-chemical reactions in liquid hydrocarbons. The present work builds on the results of experiments in the microwave discharge in liquid n-heptane [3,4] and the data, obtained by numerical two-dimensional simulation [5]. The two-dimensional model has included hydrodynamic the equations of incompressible liquid and compressible gas, the heat equation, the Maxwell's equations for the microwave field and the balance equations for the electron and n-heptane concentrations, including the gross-reaction for the decomposition of the latter. In this paper, in the framework of zero-dimensional model we present a detailed analysis of kinetic processes occurring within the gas bubbles with plasma, taking into account the formation of soot particles.

The kinetic mechanism for gas-phase reactions consists of two blocks describing the pyrolysis of n-heptane and pyrolysis of acetylene. This mechanism involves different channels of the formation and growth of polyaromatic hydrocarbons up to the pyrene molecules, which are assumed the nuclei of soot particles. The choice of the polyaromatic way of formation of soot particles was made due to the presence of the aromatic compounds in the solid phase of plasma products [3]. For the growth of solid particles we use a modified model from [6]. A surface growth of the solid particles is carried out in reactions of joining of the acetylene to the active centres on a solid surface. The coagulation of solid particles is described by the analogue of the Smoluchowski equation. Simulations includes the diffusion of gas particles to the boundary of the bubble and the inflow of n-heptane into the bubble due to evaporation. The calculation is performed at a constant gas temperature corresponding to the value obtained both in the experiments and two-dimensional modeling.

The calculations allowed us to trace the evolution of gaseous reaction products of the pyrolysis of n-heptane up to 0.01 sec - typical time of separation of the gas bubble from the electrode. The distribution function for the sizes of the soot particles is obtained. The resulting distribution function of soot particles in size up to 100 nm. Contribution of various mechanisms in forming of the distribution function for the sizes of the soot particles at different time stages is analyzed. The results of calculations and experiment are compared.

References

1. Bruggeman P. *et al* Plasma Sources Science & Techn., 2016, V. 25, 053002.
2. Lebedev Yu. A. Plasma Phys. Reports , 2017, V. 43, P. 676-686
3. Averin, K. A., Lebedev, Yu. A., Shchegolikhin, A. N., and Yablokov, M. Yu.  Plasma Processes and Polymers 2017, 14, Issue 9, DOI 10.1002/ppap.20160022
4. Lebedev Yu. A., Averin K. A., Tatarinov A. V., Epstein I. L., EPJ Web of Conferences, 2017, V. 149, 02002
5. Lebedev Yu. A., Tatarinov A. V., Epstein I. L., Averin K. A. Plasma Chem. Plasma Process. 2016, V.36, P. 535-552
6. Merkulov A. A., Ovsyannikov A. A., Polak L. S., Popov V. T., Pustilnikov V. Yu. Plasma Chem. Plasma Process. 1989, V. 9, P. 95-120