Numerical investigation of energy transfer efficiency from microwave radiation to plasma in a cylindrical resonant cavity

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Abstract. The paper presents a simplified numerical model of the hydrogen plasma generation process in a microwave resonant cavity. The model assumes electroneutrality and the prescribed electron temperature of the plasma, thus significantly reducing the computational cost. This allows for the parametric study in a wide range of operating pressures and electric field magnitudes (at a frequency of 2.45GHz). The prescribed model allows finding the effective range of operating pressures for the plasma generation. At low pressures, the collision rate is too low to effectively absorb all the emitted energy, while at high pressures the electron conductivity drops which also reduces the absorption efficiency.

1. Introduction
One of the promising directions in the development of chemical vapor deposition (CVD) [1-3] is the use of a microwave discharge to activate the mixture. The possibility of focusing the plasma potentially allows controlling the position and intensity of the discharge by changing the geometry of the resonance chamber. In this process, the estimation of the amount of microwave energy absorbed in the plasma is extremely important. The absorption coefficient can vary significantly depending on the parameters of the discharge. Experimental evaluation of the energy absorption efficiency is difficult due to the need to simultaneously control a large number of parameters. This is hard to organize in compact resonance chambers. A numerical simulation approach can help to address this problem.

In this work, a numerical model of a resonance chamber (based on experiments [2, 3]) was implemented. The discharge parameters were taken in the range suitable for plasma-assisted gas-jet diamond deposition, for a microwave (2.45 GHz) discharge within the pressure range from 10 to 400 Torr at a net supplied power of microwave radiation of 1 ÷ 5 W/cm³.

The model was implemented based on the Elmer open-source package (www.elmerfem.org) using a finite element solver with the GMRES minimum residual method. One of the main requirements for the model was the ability to estimate the fraction of the power of electromagnetic radiation absorbed in the plasma and then converted into heat, necessary for heating the carrier gas (hydrogen) and its dissociation.

The main difficulty in plasma modeling is that the time scales for the motion of electrons are significantly smaller in comparison with the time scales for the motion of heavy particles. Another difficulty is in the strong nonlinearity of the equations of plasma chemistry. In this regard, it was proposed to consider a simplified formulation to find the equilibrium distributions of the electron density. For this purpose, when constructing a computational model, several approximations were used:
1. Approximation of electroneutrality, justified by the weakness of the arising electrostatic fields in comparison with the microwave field, which has the main effect on the discharge.

2. Fixed average temperature of electrons. In a microwave discharge, the maximum electron temperature depends much weaker on the electron mean free path than in a constant field. According to estimates for a hydrogen microwave plasma, the effective electron temperature was chosen equal to 1.3 eV.[4]

The main function of the model is to convert the energy flux from microwave radiation through the distribution of electrons (conduction mechanism) into heat release in the gas. The amount of energy absorbed by electrons from the microwave field in the resonator of the experimental setup [3] was calculated for the supplied power in the range from 1 to 3 kW and hydrogen pressures ranged from 25 to 600 Torr.

2. Computation details

To find the distribution of the electric field in the volume of the discharge chamber, the vector Helmholtz equation (1) (Maxwell's equation in the time-harmonic approximation) was solved:

$$\Delta \tilde{E} - \mu \varepsilon_0 \alpha^2 \left( \varepsilon_r - \frac{i\sigma}{\omega \varepsilon_0} \right) \tilde{E} = 0,$$  \hspace{1cm} (1)

where $\tilde{E}$ is the complex amplitude of the electric field, $\mu$ and $\varepsilon$ are the magnetic and dielectric permittivities, $\omega$ is the frequency of the microwave field, $\sigma$ is the electron conductivity. The influence of electrons was set through the conductivity which was calculated from the electron density and the average collision frequency $\nu_e$ (2).

$$\sigma = \frac{q_e^2 n_e}{m_e (\nu_e + i\omega)},$$  \hspace{1cm} (2)

where $q_e$ and $m_e$ denote the charge and mass of an electron, $n_e$ is the volume concentration of electrons. For the collision frequency $\nu_e$, the following approximate expression was used [4]:

$$\nu_e = k_{Ar} n_{Ar} + k_{H2} n_{H2} + k_{H} n_{H}$$  \hspace{1cm} (3)

This expression was obtained in [4] from the solution of the Boltzmann equations for a mixture of hydrogen and argon, taking into account the main collision cross-sections. Here $n_{Ar}$, $n_{H2}$, $n_{H}$ are the number densities of argon, molecular and atomic hydrogen, respectively. The coefficients $k_{Ar}=1.8 \cdot 10^{-14}$ m$^3$/s, $k_{H2}=1.1 \cdot 10^{-13}$ m$^3$/s, $k_{H}=1.5 \cdot 10^{-13}$ m$^3$/s were taken from [4] where they were calculated for an electron temperature of 1.3 eV. This temperature was set as effective in the current calculations.

The electrons were heated through Joule losses (4).

$$Q_e = 0.5 \text{Re} \left( \sigma \tilde{E} \cdot \tilde{E}^* \right)$$  \hspace{1cm} (4)

Let us write the energy balance equation for the electrons without taking into account the Coulomb fields:

$$\frac{\partial k_b T_e n_e}{\partial t} = Q_e - n_e N \sum_i k_i(T_e) \Delta \varepsilon_i + D \Delta (T_e n_e),$$

where $N$ is the concentration of neutral molecules, $k_i(T_e)$ and $\Delta \varepsilon_i$ are the rates of electronic reactions and their energy yield, $D$ is the diffusion coefficient equal to $5/3 k_b T_e / (m_e^{*} \nu_e)$.

Under stationary conditions and fixed electron temperature, this equation can be significantly simplified as follows:

$$Q_e - n_e N k_{\text{eff}} \Delta \varepsilon_{\text{eff}} + T_e D \Delta (n_e) = 0$$  \hspace{1cm} (5)

where $k_{\text{eff}} \Delta \varepsilon_{\text{eff}} = \sum_i k_i(T_e) \Delta \varepsilon_i$. This equation has a simple form of the diffusion equation with a source and allows finding the concentration of electrons in a much shorter time than the original
system of equations. This allows conducting calculations in a wide range of parameters. The system of equations (1) - (5) sets the model for calculating the electron density, adopted at this stage of work.

To verify the model, the results of calculations based on the described model were compared with those with the drift-diffusion model from [5], with the resolution of individual evolutionary equations for the energy and concentration of electrons, taking into account the Coulomb interaction of electrons. The calculations were compared for a cylindrical resonance chamber (100 mm in diameter and 170 mm high, simulating the experimental setup), filled with molecular hydrogen, with a pressure of 50 Torr, with an input microwave radiation power of 3 kW and a frequency of 2.45 GHz. The results of the comparison of the obtained electron densities are shown in Fig. 1.

![Figure 1. Comparison of the obtained electron densities for a microwave discharge in a cylindrical resonator chamber at a hydrogen pressure of 50 Torr. (a) – calculation according to the model of the current stage, (b) – calculation in a non-stationary setting in the drift-diffusion approximation.](image)

### 3. Results and discussion

Using the model implemented at this stage, the amount of energy absorbed by electrons from the microwave field in the resonator of the experimental setup was calculated for input power, ranged from 1 to 3 kW and hydrogen pressures ranged from 25 to 600 Torr. Figure 2 shows the distributions of the released power inside the chamber for different hydrogen pressures at an applied radiation power of 3 kW. It can be seen that for low pressures, the distribution is less localized in space (which is associated with a larger value of the electron diffusion coefficient at low pressures), but has a significantly lower power amplitude. With an increase in pressure, the released power is localized near the outlet nozzle, and the power amplitude first increases with increasing pressure, and then, after ~300 Torr, begins to decrease.

Figures 2d,e,f show the distributions of the released power normalized by the electron concentration. It can be seen that, per electron, the distributions become closer in magnitude. At the same time, the normalized power increases with increasing pressure.

These patterns are reflected in the graph of the total absorbed power (as a percentage of the supplied microwave power) versus pressure (Fig. 3a, b). It can be seen from the graph that the absorbed power first increases with increasing pressure, and then begins to decline rapidly. At the same time, for all three considered input power levels, this value at the peak reaches ~70-75%. Thus, it can be seen that it is important to select the correct discharge parameters when most of the power will be absorbed in the chamber rather than reflected back into the magnetron.
Figure 2. Distributions of absorbed power (a-c) and the ratio of the absorbed power to the electron concentration (d-e) for input power of 3 kW and pressure of 25 Torr (a,d), 300 Torr (b,e), 600 Torr (c,f).

The plots for different pressures coincide when built with a value proportional to the reduced field \( \frac{E}{n_e} \), which is a characteristic parameter for the discharge process. In Fig. 3a, the ratio of the pressure to the root of the input power is chosen as such a value.

The low efficiency of absorption of microwave radiation at low and high pressures can be explained by the fact that at low pressures electrons have a lower probability of collisions with molecules and, hence, there are fewer ways to utilize the energy of the microwave field during the period of acceleration by an alternating field, while at high pressures, the number of electrons becomes too small to maintain the required conductivity, which leads to the extinction of the discharge.

Figure 3c shows a curve representing the number of electrons in the discharge chamber versus pressure, the curve is close to linear. The number of electrons decreases with increasing density at a fixed power. The degree of ionization is shown in Fig. 3d, it can be seen that it also rapidly decreases with increasing density.
Figure 3. Absorbed to input power ratio (a,b), total electron number in the discharge chamber (c), and relative electron density (d) for different pressures (for 1kW power).

The model allowed estimating the microwave radiation absorption process in the low-temperature plasma. This model is applicable for the optimization of the resonant chamber shape. It is sensitive to the main effects in the medium while relatively cheap from a computational viewpoint. The planned development for the model is to apply an algebraic model for electron temperature instead of its constant value.

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