Numerical optimization of plasma generation in a microwave resonant cavity

M Yu Hrebtov* and M S Bobrov
Institute of Thermophysics of SB RAS, 630090, 1 Ac. Lavrentyev Ave., Novosibirsk, Russia
*E-mail: weexov@ya.ru

Abstract. The paper presents a numerical simulation of the hydrogen plasma generation process in a cylindrical microwave resonant cavity at moderate pressures (10 Torr). We introduce a modification to the chamber by placing several spherical dielectrics with a high permittivity at the central axis. The radii of the spheres are chosen for the Mie resonance for microwave radiation (at 2.45GHz frequency) to occur. For a dimer configuration where two spheres are placed closely together, a maximum of the electrical field magnitude is located in the gap between the spheres where the intense discharge occurs. Positioning the spheres in different spots of the chamber allows controlling the process of the microwave plasma generation. Such modification is promising for a stable discharge initiation and for preventing the discharge breaking in the microwave cavity.

1. Introduction
Microwave plasma devices have a lot of industrial applications in different areas, such as plasma-assisted Chemical Vapor Deposition (CVD) for creating fine coatings with different materials [1-3] or microwave-discharge thruster engines for small spacecrafts [4]. The attractive feature of microwave plasma is the possibility to detach the energy deposition from the electrodes by utilizing resonant cavities that focus the radiation at some localized volume inside the cavity. This feature allows protecting the electrodes from erosion thus increasing the operational time and lowering the maintenance costs of the devices.

Recently a novel CVD technique has been proposed, in which a plasma-activated mixture formed in the microwave resonant cavity is ejected onto a substrate plate [2]. This method is promising for the application of coatings over large surface areas, which is crucial for industrial applications. The current paper aims at optimizing research of the resonant microwave plasma cavity by means of numerical simulation, mainly to improve the stability of the plasma generation and to increase the mixture temperature and hydrogen dissociation degree.

It was shown in [5] that spherically-shaped dielectrics with high permittivity and fine-tuned radii when placed closely together and subjected to a microwave radiation may amplify the microwave field in the gap between them. Such process occurs because of Mie resonance effects when the radiation wavelength inside the dielectric is a factor of a perimeter of the sphere cross-section. For a single spherical dielectric the radiation is focused in its center, while for a dimer configuration of the two spheres the scattering leads to the focus shifting outwards from the dielectric. For such configuration an intense microwave discharges were reported under atmospheric pressure in [5].
This property of focusing the microwave radiation might be very useful for CVD or other microwave plasma applications as it allows controlling the discharge initiation position and may potentially stabilize the plasma behaviour at higher pressures.

In the current paper the effect of the introduction of such spherical dielectrics with high permittivity into a cylindrical microwave chamber is studied numerically.

2. Computation details

We simulate a cylindrical resonant chamber with a diameter of 105 mm and the height of 140 mm. The chamber is split in half by a 10 mm thick quartz plate. In the upper part of the chamber a microwave coaxial antenna from the magnetron is located. At the bottom of the chamber a small nozzle is located with the jet outlet orifice (1 mm in diameter). Small inlet nozzles are located below the quartz plate. This setup is mimicking the experimental configuration from [2]. For the working fluid molecular hydrogen is chosen (which is the main part of the mixture for a diamond deposition process). The geometrical dimensions are taken for the entire chamber to have a microwave resonance frequency of 2.45 GHz.

\[
\Delta \vec{E} - \mu \varepsilon_0 \omega^2 \left( \varepsilon_r - \frac{i \sigma}{\omega \varepsilon_0} \right) \vec{E} = 0
\]

\[
\sigma = \frac{q_e^2 n_e}{m_e \left( v_e + i \omega \right)}
\]

\[
Q_{e} = 0.5 \text{Re} \left( \sigma \vec{E} \cdot \vec{E}^* \right)
\]

For the numerical model, we use time-harmonic Maxwell equation (1) for the microwave part, assuming that the frequency of the microwave radiation is fixed (at 2.45 GHz). Here \( \varepsilon_r \) denotes relative permittivity, \( \omega \) is the radian frequency and \( \sigma \) is the conductivity of the plasma. For the walls of the chamber we use perfect conducting conditions. Quartz (\( \varepsilon_r = 4.5 \)) and water (\( \varepsilon_r = 79 + i10 \)) dielectrics are used. The imaginary part of permittivity of the water is used to simulate dielectric losses.

For the plasma part of the simulation a drift-diffusion approximation is used with electron impact reactions rates taken from the experimental cross-sections data (Table 1).

| Reaction | Type       | Cross-section data source |
|----------|------------|---------------------------|
| \( e + H_2 = e + H_2 \) | Elastic collision | [6] |
| \( e + H_2 = 2e + H_2^* \) | Ionization | [7] |
| \( e + H_2 = e + 2H \) | Dissociation | [7] |
| \( e + H = e + H \) | Elastic collision | [7] |
| \( e + H = 2e + H^* \) | Ionization | [7] |

The coupling between microwave and plasma equations was done through heating of the electrons by microwave radiation (3) and through the electron conductivity relation in plasma (2). The equations were solved with the finite element simulation package COMSOL Multiphysics in axisymmetric formulation.

At the chamber boundaries the recombination surface reactions were used to restore the original mixture composition. The boundaries were assumed grounded. At the dielectric boundaries an insulation conditions were set.
The simulations were carried out the equilibrium concentrations of electrons and heavy species were set in the simulation domain. Due to low ionization rates for the used (1 kW) power of the microwave source the bulk recombination was assumed much weaker than its surface counterpart.

The simulation parameters are shown in Table 2.

| Parameter       | Description                  | Value  |
|-----------------|------------------------------|--------|
| \( p_0 \)       | Chamber Pressure (Torr)      | 100    |
| \( P_{\text{dep}} \) | Radiated microwave power (W) | 1000   |
| \( n_e^0 \)     | Initial electron density (m\(^{-3}\)) | \( 10^{16} \) |
| \( T_e^0 \)     | Initial electron temperature (eV) | 1      |
| \( n_{\text{H}_2} \) | Initial \( \text{H}_2^+ \) concentration | \( 10^{16} \) |
| \( x_n^0 \)     | Initial H mole fraction      | \( 10^{-8} \) |
| \( f \)         | Microwave frequency (GHz)    | 2.45   |

All the species were considered isothermal except for the electrons. So, the thermal dissociation of hydrogen molecules was not taken into account. While the thermal dissociation may be the main source of atomic hydrogen on longer time scales including it into the simulation would significantly slow down the computation. As the main focus was to study the effects of dielectrics on plasma generation the thermal dissociation was omitted.

**Figure 1.** The microwave electrical field distribution for the baseline case (a); case with single sphere (\( s=4 \)) (b); and case with two spheres (\( s=2 \)) (c).
The presented simulations might be considered as the initial stage of the discharge where the thermal effects are not yet significantly pronounced in the heavy species transport. Still the simulations can show the difference in the discharge regime of different modifications of the microwave resonant chamber.

3. Results and discussion

3.1. Effects of the dielectric on the microwave field

At first the microwave part (1) without plasma equations was simulated to see how the electrical field will be redistributed after the addition of spherical dielectrics. Mie resonance conditions for the spherical dielectric should be valid if the perimeter of the circle cross-section of the sphere contains an integer number of the wavelengths inside the dielectric. Following [5] we used water (with refraction index \( n=8.9 \)) as a dielectric for the spheres. Our simulations have shown that for effective perimeter \( (s=2\pi r n / \lambda) \) of \(~2\) and \(~4\) there is a substantial resonance effect inside the dielectric. For a single sphere the most prominent effect is observed for \( s=4 \) which translates to \(~1\) cm radius of the sphere. For this case the field is concentrated at the center of the dielectric sphere. This means that most of the energy will be dissipated through the dielectric losses inside the sphere.

For the configuration with two closely placed dielectric spheres it was found that smaller spheres with \( s=2 \) having only 2 wavelengths on the perimeter of the dielectric produce the most prominent effect of the focusing in the gap between the spheres. The optimal radius of the spheres was \(~0.4\) cm and the maximum gap that still produces a strong focusing effect was \(~2\) mm. This was considered a more promising configuration for practical purposes than the case with larger spheres (\( s=4 \)) because it has much lower dielectric losses which leads to less heating and more durable setup.

As we considered only the axis-symmetrical configurations, we could not study different mutual orientations of the dielectric spheres which would require 3D simulations. Only axial direction of the dimer was considered. Changing the axial direction of the dimer’s position led to small variation in the electrical field strength. The field was stronger if the dimer was placed farther from the center of the chamber. For practical purposes it was assumed that the most efficient position of the dimer for plasma discharge should be as far from the metallic walls as possible to minimize the charge diffusion through the conducting walls. Thus, the configuration with the dimer position below the quartz plate was considered for further simulation with plasma equations included.

We should note that in principle it is possible to change the position of the dimer in order to control the position of the discharge and focusing of the electrical field during the device operation which may be convenient for tuning the chamber for particular properties.

3.2. Effects of the dielectric on the electron density

In the second part we considered the coupled microwave-plasma simulations. For this part we only considered two cases. One with an empty chamber and the other with the ‘optimal’ dimer with spheres having effective perimeter \( s=2 \), that is described above.

For baseline cases it can be seen that plasma formation is concentrated at the bottom part of the chamber where the microwave electrical field has maximum intensity. However, the round shape of the discharge is indicative of a significant charge and electron energy loss at the metal walls of the chamber.

For the modified case with dielectric spheres the electron concentration is much less uniform and concentrated in the space between the dielectric spheres where the maximal local concentration is \(~10\) times higher than in the case of the empty chamber. The mean electron temperatures in both cases are similar and close to \( 1.1 \) eV.

While the local differences between the electron concentrations are obvious it is also important to see how the dielectrics affect the concentrations averaged over the chamber’s volume. The integration demonstrated that for unmodified case averaged electron concentration was \(~3\cdot10^{16} \) m\(^{-3}\) and for the modified case it was \(~3.5\cdot10^{16} \) m\(^{-3}\). The net growth of the electron concentration by the modification was \( 17\% \).
Further investigation is needed for more than two spheres configuration and the optimal mutual positioning of the spheres in 3D which might give more focusing effect than the current setup.

![Electron concentration distribution for the case with two dielectric spheres (s=2) (a); and the baseline case (b).](image)

**Figure 2.** Electron concentration distribution for the case with two dielectric spheres (s=2) (a); and the baseline case (b).

**Conclusion**

The current simulation shows that the inclusion of dielectric spherical dimers in the microwave discharge chamber may aid to control the plasma formation and to stabilize the discharge in microwave plasma reactors. The glass (e.g. quartz glass) spheres filled with water may be considered as a practical variant of such modification. Due to small diameters of the spheres the dielectric losses are also small compared to the conductive losses in the plasma. To prevent the overheating of the spheres the circulation cooling may be organized by adding small tubes for water circulation through the spheres. Further investigation is needed to find the optimal configuration in three-dimensional setup.

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