Machine-Learning Efficiency Optimization of Microwave Applicators with Plasma

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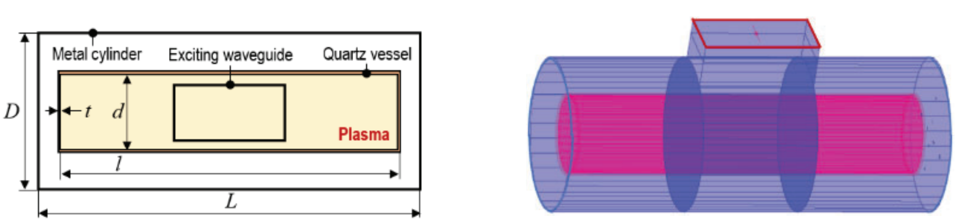
Microwave (MW) plasma has shown a significant contribution to applications in processing technology [1] with demonstrable impact on the efficiency and quality of various processes. Examples include production of synthetic diamonds [1]-[3], surface processing for semiconductor manufacturing (deposition, etching, cleaning) [1], [4], plasma-based decomposition of CO_2 [5], etc. However, advancement of these applications is constrained by the challenges associated with development of efficient and controllable MW applicators for industrial use [1].

While sample computer simulations aiding in the design of such applicators have been reported in [2], [4], [6], [7], the use of advanced electromagnetic (EM) modeling and CAD remains limited due to the absence of adequate input data for the models of the system with plasma medium. The direct measurement of complex permittivity of plasma is challenging [8], [9] and, moreover, parameters of plasma are usually specific to the MW system in which it is ignited and maintained. Therefore, the complex permittivity of plasma is mostly estimated by theoretical calculation [8]. Recently, a simple physics-driven approach to characterization of MW plasma for EM modeling using the FDTD technique was proposed in [10]. In this model, the complex permittivity of plasma is represented by the electric conductivity, which is conditioned by the plasma frequency f_p, and the frequency of electron collisions, γ. Using this approach, EM modeling of a conventional MW applicator displayed well-known behavior of the electric field in presence of plasma [10].

Presently developing this work, we propose a machine-learning (ML) technique in which an FDTD model of a MW applicator with plasma is employed in an optimization loop. This technique allows one to find the optimum geometry of the applicator and determine the neutral gas required for optimal performance. Optimality here means energy efficiency; the objective function is defined as a minimum value of the reflection coefficient $|S_{11}|$ at an operating frequency f_0. The procedure is based on the neural network technique featuring constrained optimization response surface sampling in the dynamic training of the decomposed radial-basis-function (RBF) network [11]. To demonstrate functionality of the optimization technique, we use a model of a conventional MW applicator, like that which was used in the study [10]. The model consists of a cylindrical cavity with a coaxial thin-wall quartz vessel containing uniformly distributed plasma (Fig. 1); the model is built in the 3D FDTD EM simulator QuickWave [12]. The ML procedure identifies the geometry of the applicator and the plasma parameters f_p and γ which satisfy the objective function.

In accordance with [10], plasma frequency f_p, is conditioned by electron density which, in turn, depends on the neutral gas density and the degree of ionization [4]. It is difficult to determine the specific value of electron density, however, it can be assumed within a certain plausible range. As such, we specify f_p as the design variable in our optimization procedure. Furthermore, following [10], the frequency of electron collision g, depends on the neutral gas density, the average electron velocity, and the electron collision cross-section. Per the approach [4], the first two parameters can be assumed constants. To estimate the latter, one can use the calculated atomic radius of the neutral gas in which the plasma is excited and maintained. Then γ can be seen as dependent on the gas, therefore, constituting a set of typical gases as a discrete design variable in our optimization.



(a) (b)

Fig. 1. 2D (a) and 3D (b) views of the modelled cylindrical cavity with a coaxial quartz vessel (containing plasma); contrary to [10], the cavity is excited by a longitudinally oriented rectangular waveguide.

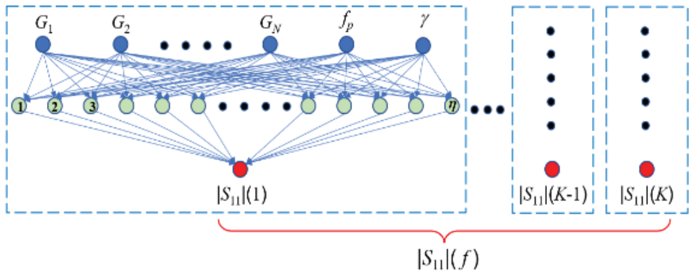


Fig. 2. Architecture of a decomposed RBF network with h hidden neurons.

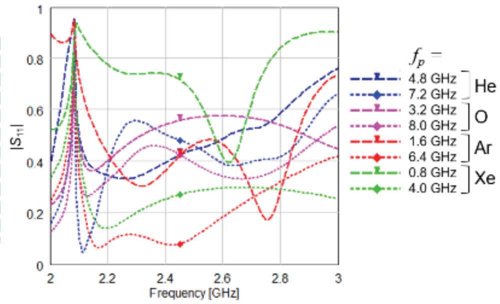


Fig. 3. Examples of non-optimal characteristics of $|S_{11}|$ for different neutral gases (γ) and plasma frequencies f_p as well as random D and d; optimized characteristic is found for Ar, f_p = 6.4 GHz, D = 95 mm, and d = 46 mm.

The RBF network used in the proposed machine-learning procedure (Fig. 2) follows the concept and methodology of the neural network optimization of microwave systems that is described in [11]. It works with input vectors of design variables $X_i = [G_1, G_2, \ldots, G_N, f_p, \gamma]$, where G_j ($j = 1, \ldots, N$) are geometrical parameters of the modeled applicator, and $i = 1, \ldots, P$, where P is the number of points (input-output pairs) of modeling data. The network output vectors are obtained by taking K equally spaced values of frequency characteristics of $|S_{11}|$ over a specified frequency range. The procedure implemented in MATLAB includes the dynamic network training and testing performed with the use of the input data for the FDTD model and its output results.

In the illustrative optimization, the applicator in Fig. 1 is characterized by constant parameters t = 1.5 mm, l = 220 mm, L = 240 mm and excited by WR284. The CAD goal is to find the values of four design variables, two geometrical parameters $G_1 = D$ and $G_2 = d$ as well as f_p and g corresponding to a minimum value of $|S_{11}| \leq 0.1$ at f_0 = 2.45 GHz. The following specifications are applied: $90 \leq D \leq 130$ mm, $40 \leq d \leq 80$ mm, $0.4 \leq f_p \leq 8.0$ GHz, and γ = [0.248 (He), 0.373 (Ne), 0.456 (F), 0.595 (O), 0.810 (N), 1.303 (Ar), 2.001 (Kr), 3.014 (Xe)]. The procedure starts with an initial database of 50 randomly chosen points generated in the specified domain, and the stopping criterion is set for the database size reaching 500 points. The FDTD model features a fine non-uniform mesh with 2 mm cells in air and 1.5 mm cells in quartz and plasma. When run on a regular Windows PC, the steady state is reached within a few minutes.

An optimized frequency response of $|S_{11}|$ is shown in Fig. 3 along with seven examples of typical non-optimized characteristics. The curve with the lowest value (0.75) of the reflection coefficient at 2.45 GHz corresponds to the specific geometry, neutral gas, and plasma frequency. The optimal design is found with 102 points in the database.

The described ML procedure employing the decomposed RBF network with three continuous (D, d, f_p) and one discrete (γ) input parameters (design variables) demonstrates its robustness and computational efficiency. The underlying FDTD model, however, relies on the simplified characterization of complex permittivity of plasma that, in particular, assumes that plasma frequency is a controllable/known parameter. With the uncertainties in input data of the EM models, our optimization procedure can be instructive in determining the operational bounds of applicators with MW plasma.

References

[1] L. Bardos and H. Barankova, *Microwave Plasma Sources and Methods in Processing Technology*, Hoboken, NJ: IEEE Press/Wiley, 2022.
[2] F. Silva, K. Hassouni, X. Bonnin, and A. Gicquel, Microwave Engineering of plasma-assisted CVD reactors for diamond deposition, *J. of Physics: Condensed Matter*, vol. 21, no. 36, 364202, 2009.
[3] E.L.H. Thomas, L. Gines, S. Mandal, G.M. Klemencic, and O.A. Williams, A simple, space constrained NIRIM type reactor for chemical vapour deposition of diamond, *AIP Advances*, vol. 8, 035325, 2018.
[4] S. Pauly, A. Schulz, M. Walker, M. Gorath, K. Baumgärtner, and G. Tovar, "Modeling and experimental study of remote microwave plasma source for high-rate etching," *Chemie Ingenieur Technik*, vol. 94, pp. 410-416, 2022.
[5] M.Y. Ong, S. Nomanbhay, F. Kusumo, and P.L. Show, Application of microwave plasma technology to convert carbon dioxide (CO_2) into high value products: A review, *J. of Cleaner Production*, vol. 336, 130447, 2022.
[6] G. Shivkumar, S.S. Tholeti, M.A. Alrefae, T.S. Fisher, and A.A. Alexeenko, "Analysis of hydrogen plasma in a microwave plasma chemical vapor deposition reactor," *J. of Applied Physics*, vol. 119, 113301, 2016.
[7] L. Latrasse, M. Radoiu, T. Nelis, and O. Antonin, "Self-matching plasma sources using 2.45 GHz solid-state generators: microwave design and operating performance," *J. Microwave Power and Electromag. Energy*, vol. 51, pp. 237-258, 2017.
[8] G. Wang, H. Pan, S. Lai, Y. Zhou, L. Wu, H. Zhu, and Y. Yang, "Dynamic measurement of relative complex permittivity of microwave plasma at atmospheric pressure," *Processes*, vol. 9, 1812, 2021.
[9] L. Li, H. Hu, P. Tang, B. Chen, and Z. He, "A microwave reflection method to determine the complex permittivity of time-varying plasma," *Proc. 2018 IEEE Intern. Symp. on Antennas and Propagation, Boston, MA, 2018*, 978-1-5386-7102-3.
[10] C.E. Williams and V.V. Yakovlev, "Characterization of microwave plasma in electromagnetic modeling for processing applications," *Proc. 57th IMPI's Microwave Power Symp., Denver, CO, June 2023*, pp. 51-53.
[11] E.K. Murphy and V.V. Yakovlev, "Neural network optimization of complex microwave structures with a reduced number of full-wave analyses," *Intern. J. of RF & Microwave Computer-Aided Engng*, vol. 21, no 2, pp. 279-287, 2011.
[12] *QuickWave*, QWED Sp. z o.o., 1998-2023, http://www.qwer.eu.