Development of a Graphical User Interface for Reflection Loss Calculation in Perovskite-RGO based Microwave Absorbing Composites

Aayushi Arya
Department of Electrical Engineering, Indian Institute of Technology Hyderabad, India
aayushi.arya@outlook.com
(corresponding author)

Received: 7 November 2022 | Revised: 24 November 2022 | Accepted: 9 December 2022

ABSTRACT

In this paper, a novel method is investigated wherein the theoretical and mathematical analysis of the perovskite-Reduced Graphene Oxide (RGO) based composite microwave absorber is used to form a machine learning model using linear regression to predict the reflection loss and the effective dielectric permittivity of a selected perovskite compound in an RGO-based composite. At first, the theoretical derivation is carried out to find a mathematical relationship between the reflection loss and the dielectric permittivity of the composite and the cationic radii of the perovskite structure, which is then used to form the base for the machine learning model to directly calculate the microwave absorption characteristics from the atomic parameters of the given composite structure. Linear regression is used for the machine learning algorithm which is verified with an R^2 of 0.869 with the atomic radii as the input parameters. The model is further used to develop a Graphical User Interface (GUI) to make the prediction more appealing and user-friendly. The current paper provides a new approach to the integration of theoretical knowledge with advanced computing tools to form innovative predictive tools for current microwave-absorbing materials.

Keywords-atomic radius; microwave absorbers; machine learning; perovskite; reflection loss; reduced graphene oxide

I. INTRODUCTION

Microwave absorbing composites have become an important field of research due to their growing applications. This field has seen a variety of research articles dedicated to the experimental studies of the absorbing properties of microwave absorbers [1-3]. There are many theoretical works also, modeling the permittivity and permeability of microwave absorbers [4-7], but they do not analyze their atomic fundamentals. In this work, an effort was conducted to form a machine learning model based on a theoretical framework for a microwave absorber that directly relates the refection loss to the atomic radii of the elements in the observed compound. Further, a Graphical User Interface (GUI) was developed for predicting the reflection loss of perovskite-Reduced Graphene Oxide (RGO)-based microwave absorbing composites from their ionic radii using the machine learning model. The base equation and the electromagnetic parameters for the model are theoretically evaluated for the given absorber composite. The considered parameters include the combined dielectric permittivity of the filler and matrix material also referred to as the effective dielectric permittivity, the effective magnetic permeability, the radius of the filler particles considered as spherical inclusions, and the effective radius of anion and cation in the perovskite unit cell.

In this work, a pervoskite-reduced graphene-based microwave absorbing composite is considered. A combination of perovskite filler and RGO-based matrix was chosen as the microwave absorbing composite. Pervoskites are chosen as filler materials due to their good electrical and magnetic properties along with physical and chemical stability [8]. Similarly, RGO has gained popularity in microwave absorbing composites replacing the conventional polymer-based matrix materials [9], due to its high conductivity and excellent physical and chemical properties. Having the advantage of increased point defects and attached functional groups, RGO facilitates the occurrence of interfacial polarization and enhanced polarization sites thereby increasing the overall absorption rate. For an effective microwave absorption in a composite, there has to be good impedance matching for maximum wave absorption followed by high dissipation of the absorbed energy. The given model can be used to form new and efficient perovskite-based microwave absorbing compounds. Perovskite-based absorbers are cost effective, non-toxic, and environmentally friendly. Hence, they can be widely used as microwave absorbers in applications with large human contact like schools, hospitals, etc. They can be applied as microwave absorbing paints, coats, or integrated with absorber foams.

II. POLARIZATION AND MAGNETISM

Polarizability is the tendency of an atom to allow charge separation when exposed to an electromagnetic wave. There are different polarization kinds that can occur inside a composite system including electronic, ionic, interfacial, and dipole relaxation-based polarizations [10-12]. As depicted in Figure 1(a), for a perovskite and graphene-based composite absorber, all the above phenomena happen at different points resulting in strong EM wave absorption. Dipole polarization occurs across the graphene layers due to the relaxation of dipoles formed between the graphene layers that are loosened with the penetration of perovskite particles between them. Similarly, in ABO3-type perovskite structures, ionic polarization occurs at the oxide ions formed by the presence of positively charged A-site cation deficiency. Interfacial polarization is induced by the interaction of the A-site cation with the matrix material that is graphene. This is caused by the interaction across a heterogeneous boundary creating a charge separation on both sides of the boundary. Electronic polarization is attributed to the flow of oxide ions in the 2D and 3D layers across the perovskite particles. The 2D oxide ion conduction occurs across the B-O-B plane, however the introduction of the graphene matrix between the perovskite structure has enabled 3D movement of the oxide ion. Graphene forms interfacial polarization with the A-site cation hence weakens its restricting force over the movement of oxide ions from one-unit cell to another. This phenomenon results in the formation of electronic polarization as well.

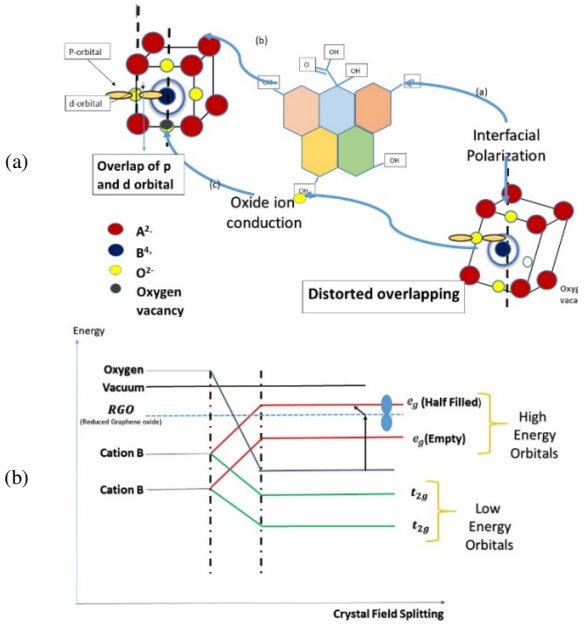

Fig. 1. (a) Polarization mechanism, (b) energy band diagram showing the occurrence of magnetism in perovskite-RGO composite microwave absorber.

The occurrence of magnetism in a perovskite compound occurs via double charge mechanism and involves the influence of RGO which forms a boundary material across the perovskite. The spin coupling in the perovskite filler particles is supported by the RGO layer. As shown in Figure 1(b), cation A is not disturbed by the bond formation and provides a higher single energy level. On the other hand, cation B when combined with oxide ion and forming a B-O-B bond, splits its energy level into higher (e_g) and lower (t_{2g}) [13] energy orbitals. In a well ordered perovskite structure, the d-orbital of the B cation overlaps with the p-orbital of the oxide ion in a covalent manner with equal charge distribution. However, due to the presence of an additional energy level of RGO, the octahedron perovskite structure shifts from its center of symmetry. The perovskite oxide can show either ferromagnetic or magnetic properties when the electron charge distribution in the B-O-B bond is such that, one of the B cations is empty while the other is half filled following Goodenough-Kamamori's rule on superexchange interactions [14-15], thus increasing the overall magnetic permeability of the compound [23-24].

III. THEORETICAL FRAMEWORK

The effective relative permittivity can be calculated from the Maxwell Garnett equation [16]:

$$\varepsilon_{eff} = \varepsilon_m \frac{2\delta_i(\varepsilon_i-\varepsilon_m)+\varepsilon_i+2\varepsilon_m}{2\varepsilon_m+\varepsilon_i-\delta_i(\varepsilon_i-\varepsilon_m)} \quad (1)$$

The dielectric permittivity for the matrix material (RGO) is taken as constant, $\varepsilon_m = 118$. The maximum value of the dielectric constant is taken to compensate for the high temperature effects on account of the dissipation of the absorbed microwaves [17]. The volume fraction of the filler particles is taken as the critical percolation threshold for the filler particles in an infinite cubic lattice. Its value is 0.1454 in all three dimensions [18]. Similarly, the effective relative magnetic permeability (μ_{eff}) can be calculated from [19]:

$$\mu_{eff} = \mu_d \left(1 + \frac{\delta_i}{10}\frac{\omega^2}{c^2}\left(a_{pc}\right)^2 \varepsilon_m\right) \quad (2)$$

where a_{pc} is the atomic radius of the filler inclusions. In this case it is taken as the pseudo cubic lattice constant of the perovskite structure [25].

To determine the pseudocubic lattice constant a_{pc} of the perovskite filler particles, the effective anion radius, accounting for the effect of oxygen vacancies must be calculated which in turn should be determined from an estimated size of the spherical filler particles from the given dielectric permittivity [20]. The atomic size of the filler particles which are assumed to be spherical can be calculated by the Claussius Mosotti equation:

$$\alpha = \left(\frac{\varepsilon_i-1}{\varepsilon_i+2}\right) a^3 \quad (3)$$

The value of α is taken as 2.36×10^{28} from [13] on the theoretical predictions of electric and magnetic parameters of microwave absorbers.

Rearranging (6), it can be rewritten as:

$$a^3 = \alpha\left[\frac{\varepsilon_i}{\varepsilon_i-1} + \frac{2}{\varepsilon_i-1}\right] \quad (4)$$

In (7), the first term accounts for the effect due to the electronic polarizability, while the second term represents the effect due to the dipole polarizability. Since the dipole

polarization is the dominant at microwave frequencies, the first term can be dropped giving the modified equation for the atomic radii of the spherical filler inclusion as:

$$a = \sqrt[3]{\alpha \left[\frac{2}{\varepsilon_i - 1}\right]} \quad (5)$$

This approximated value is used to calculate the effective oxygen anion radius in the perovskite unit cell:

$$r_{x_{eff}} = \frac{a}{2} - r_b \quad (6)$$

The overall pseudo cubic lattice constant of the perovskite structure can be calculated as:

$$a_{pc} = K(V_N)^S r_{av} \quad (7)$$

where $V_N = V_A V_B V_X$ is the product of the valence electron of cations A and B and O anion respectively. Similarly r_{av} is the average of the atomic radii of the A, B, and O atoms. K and S are constants with values 2.45 and 0.09 for cubic pervoskites. Equation (7)is used to find the effective magnetic permeability from (2). Effective permittivity and permeability are further used to calculate the input impedance of the absorber as follows:

$$Z_{in} = \sqrt{\frac{\mu_{eff}}{\varepsilon_{eff}} \frac{\mu_o}{\varepsilon_o}} \quad (8)$$

where μ_o and ε_o are the permeability and permittivity of free space respectively. After finding all the above parameters, the final Reflection Loss (*RL*) is calculated by:

$$RL = 20\log\left(\frac{Z_{in} - Z_o}{Z_{in} + Z_o}\right) \quad (9)$$

where Z_o is the characteristic impedance of the input medium taken as free space.

IV. MACHINE LEARNING MODEL-LINEAR REGRESSION

The multiple linear regression model is used to relate the *RL* which is the most important absorption characteristic of an absorber to the fundamental value of an atom that is its atomic radius. A plot between the cationic radii and the *RL* is presented in Figure 2 suggesting an almost linear relationship between the output and the input parameters. The straight lines connecting the different data points and the shaded area indicate the change in *RL* with the change in individual atomic radius. The flowchart in Figure 3 shows the flow of the given work and how the different parameters are ultimately fed to the machine learning algorithm. In order to first apply the multiple linear regression model, the validation of the significance of the input features is conducted by applying the Ordinary Least Square (OLS) method. There are two results in the OLS model summary that are of interest, the coefficient of determination (R^2) and the p-value. R^2 measures the amount of variation in the output feature captured by the corresponding variations in the input parameters while the p-value provides a conditional probability of a null output hypothesis.

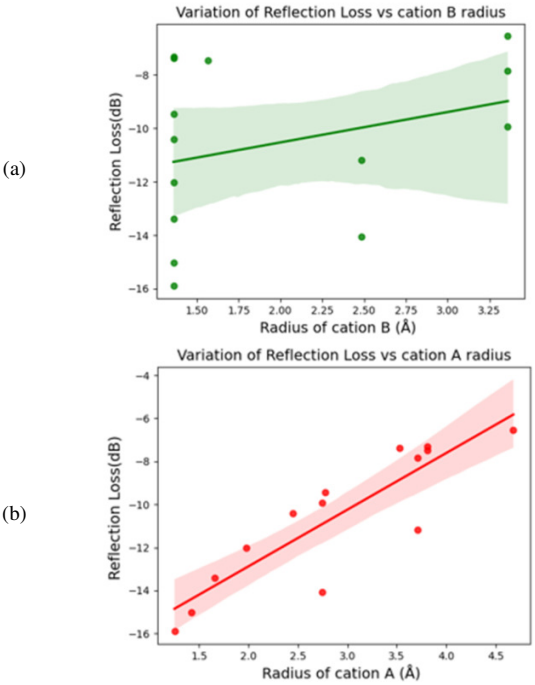

Fig. 2. Linear relationship between the *RL* and the cationic radii.

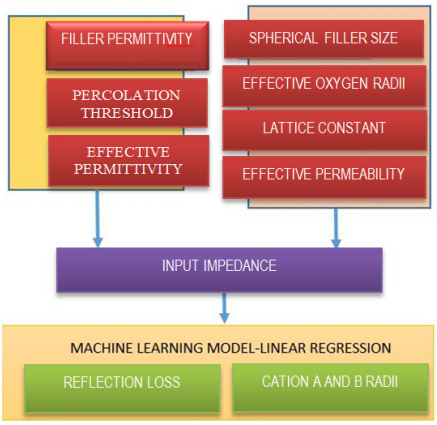

Fig. 3. Step flow and parameter merging of the machine learning algorithm.

If the p-value is less than 0.05, the input features do not fulfil the null hypothesis. In the OLS model summary for the current model, both the above two requirements are met, thus both of our input features have significant effect on the output and can be successfully used in a linear regression relation with the output. After validating the parameters, multiple linear regression is applied. The linear regression forms a linear equation between the input and the output parameters and provides the intercept with the coefficient of the individual input parameters. From the given equation, *RL* can be predicted for the given dataset, and can be compared with the actual result. Table I describes the dataset [20] for the various ABO3 type perovskite materials with their respective permittivity values. This dataset was used for the calculations and the formation of the empirical results.

TABLE I. INPUT AND CALCULATED ELECTROMAGNETIC PARAMETERS OF PERVOSKITE STRUCTURES

Material	ε_i	r_a	r_b	r_{av}	ε_{eff}	a	V_N	a_{pc}	μ_{eff}	Z_{in}	RL	RL_{pred}
$CaTiO_3$	160	10.99	9.94	2.31	1170	1.437	48	8.022	3893.957	687.12	-14.07	-11.33
$CaZrO_3$	27	10.99	16.79	2.71	957.3	2.628	48	9.4	5346.693	890.31	-9.93	-11.97
$SrZrO_3$	30	18.57	16.79	3.32	964.1	2.534	48	11.524	8035.893	1087.63	-7.84	-9.13
$BaZrO_3$	35	28.07	16.79	3.92	975	2.403	48	13.607	11203.44	1277.02	-6.55	-6.28
$LaGaO_3$	27	22.86	6.26	3.42	957.3	2.628	54	11.984	8690.231	1135.05	-7.47	-7.53
$SrTiO_3$	300	18.57	9.94	2.86	1292	1.164	48	9.941	5979.781	810.4	-11.19	-8.49
$NdAlO_3$	22.5	14.68	4.08	2.57	947	2.8	54	8.998	4899.176	856.86	-10.42	-11.59
$LaAlO_3$	23	22.86	4.08	3.47	948.2	2.779	54	12.159	8945.896	1157.14	-7.31	-7.38
$PrAlO_3$	23	16.67	4.08	2.78	948.2	2.779	54	9.746	5747.551	927.5	-9.45	-10.42
$ErAlO_3$	16	7.51	4.08	1.89	931.6	3.157	54	6.62	2651.9	635.6	-15.9	-14.91
$DyAlO_3$	18	8.56	4.08	1.96	936.4	3.028	54	6.876	2860.948	658.49	-15.02	-14.4
$GdAlO_3$	18	9.94	4.08	2.11	936.4	3.028	54	7.416	3327.942	710.19	-13.39	-13.72
$SmAlO_3$	20	11.85	4.08	2.29	941.2	2.918	54	8.034	3905.686	767.42	-12.03	-12.78
$YAlO_3$	16	17.64	4.08	3.40	931.6	3.157	54	11.942	8629.466	1146.57	-7.38	-8.21

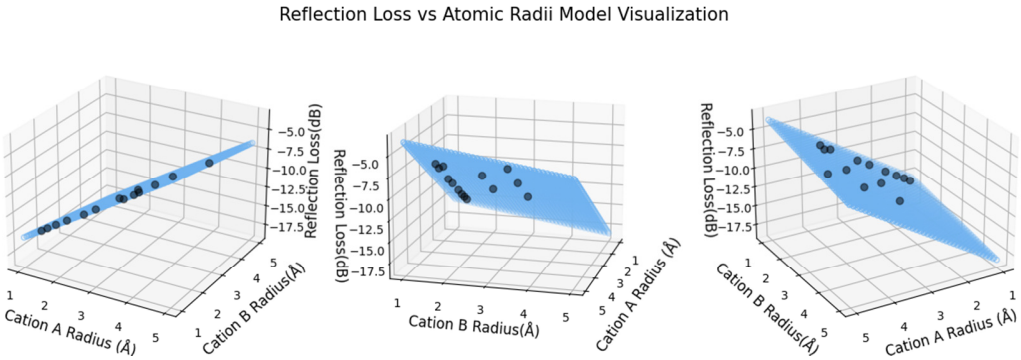

Fig. 4. 3-D model visualization of the given machine learning model.

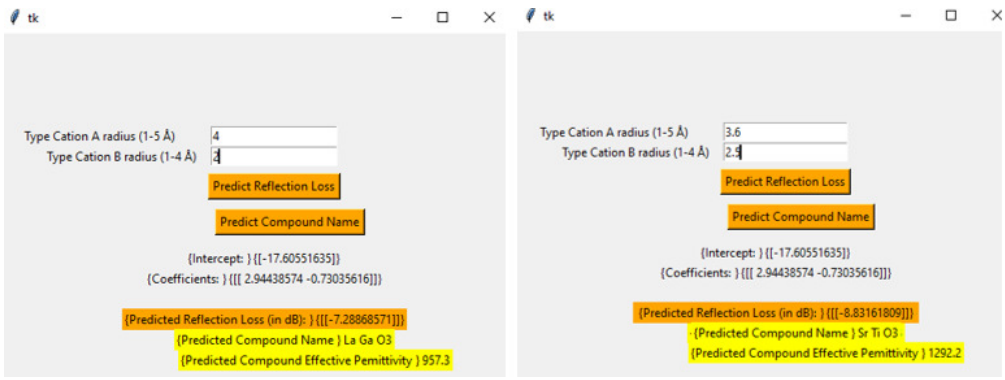

Fig. 5. The developed GUI.

All the values provided in Table I are used to calculate the various electromagnetic parameters derived in the previous theoretical framework which are also tabulated in Table I along with the theoretical and predictive values of the *RL*.

3D graphical visualization of the variation in the *RL* with respect to cation A and B radii is presented in Figure 4. The inclusion of the two cationic radii as input variables provides a rectangular model area, which covers all the data points provided for model training. The data plots are well contained within the model scope. From the given machine learning model, a GUI is developed, as shown in Figure 5, for the calculation of the *RL* of the perovskite compound and its effective permittivity based on the atomic radii provided by the user. The GUI takes the cations' A and B radii as input and suggests a suitable microwave absorbing perovskite compound. It also shows the output *RL* and the effective permittivity based on the machine learning predictive model. The GUI is tested by taking two sets of input atomic radii and the output results are matched with the results of Table I. The results are in good accordance showing the high accuracy of the developed GUI.

TABLE II. MODELING PARAMETERS OF THE PROPOSED LINEAR REGRESSION MODEL

Intercept	Coefficients
-17.605	[-2.944 -0.73]

V. CONCLUSION

In the present work, a new and innovative method has been suggested of utilizing a theoretical framework to develop a machine learning GUI for estimating the reflection loss in microwave absorbers. This work includes the diverse mechanisms and phenomena working behind the application of microwave absorption in a single equation using machine learning tools. This helps not only the simplification of the accurate calculation of reflection loss without going into huge depths of the physical processes of polarization, magnetism, and dissipation across the absorber, but also opens a new window to develop advanced software and algorithms devoted to the formation of new and complex kinds of microwave absorbers. Using this approach, the microwave absorber can become a part of more general engineering. It is time we take advantage of the true potential of microwave absorbers because such materials can be used for the benefit of society, as in hospitals, schools, libraries, etc. reducing the harmful effects of the EM wave radiation exposure in the ambient surroundings.

VI. DATA AVAILABILITY STATEMENT

The data that support the findings of this study can be accessed at [22].

NOMENCLATURE

Parameter	Notation
Effective relative permittivity	ε_{eff}
Effective relative permeability	μ_{eff}
Filler permittivity	ε_i
Radii of the spherical filler particle	a
Effective radius of oxygen anion	$r_{x_{eff}}$
Pseudo cubic Lattice constant	a_{pc}
Volume fraction of filler inclusion	δ_i
Product of valence electron of cation A, B, and O	$V_N = V_A V_B V_X$
Average atomic radius of the A, B, and O atoms	r_{av}
Input impedance of the absorber	Z_{in}
Reflection Loss (dB)	RL

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AUTHORS PROFILE

Aayushi Arya is currently pursuing her Phd from the EE Department, Indian Institute of Technology, Hyderabad, India. With keen interest in fundamental and physical concepts, I have done research works in deriving the theoretical and mathematical framework of microwave absorbers followed by the integration of the derived concepts in advanced modeling tools such as machine learning.