Prediction of material composition for microwave absorption through mathematical modelling

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Abstract
In this paper, we analyse the suitability of various elements and their composition for microwave absorption. This is done by developing a mathematical model based on transmission line theory, polarizability and dielectric and magnetic response of the material. The inputs to this model are the desired specifications of the absorber like reflection loss, resonance frequency and bandwidth. The corresponding output parameters are the range of the atomic radii and magnetic dipole moment of suitable elements and their effective energy parameters. This mathematical model has been verified for compounds like oxides and ferrites that have been proven to possess microwave absorption properties through previous experimental research. This mathematical model has been verified for compounds like oxides and ferrites that have been proven to possess microwave absorption properties through previous experimental research. Through numerical computations, we propose new material compositions with various elements that can be used as effective microwave absorbers.

1. Introduction

Microwave Absorbers have become very popular in recent years, owing to their immense potential for applications like wireless circuitry and RF communication. With a continuous increase in the use of Electromagnetic wave radiations, microwave absorbers has now become a necessity in areas like wireless communication, Electronic Devices and others. A vast amount of literature can be found on experimental verification of new materials and compounds as microwave absorbers. However with less amount of theoretical research and background in the area, the experimentations are more based on previous findings leading to a hit and trial methodology. Thus in this paper we attempt to present a theoretical model based on several theories of microwave absorption to form a predictive model for selection of new and different elements and compounds that can provide efficient microwave absorption. The model extracts a suitable range of atomic radii and magnetic dipole moments from which different elements can be selected as cations. The elements are further used to form a microwave absorbing compound by using empirical formulations based on their effective energy parameter which is a measure of the polarization tendencies of the individual elements, valency and other atomic parameters.

1.1. Description of theoretical calculation
A Microwave Absorber can be analysed by mathematically modelling its wave absorption and dissipation phenomenon. The absorption in dielectric based absorbers can be understood by Transmission Line Theory and dielectric polarization. The polarization capacity of each constitutive element of the material compound affects the efficiency of the absorber. For predicting a suitable range of atomic radii for the absorber composition, the polarization and the dielectric properties of the absorber have been extracted [1–5]. As shown in the flowchart 1 Three mathematical flows have been used one using the transmission Line theory, another using the polarisation theory and the third one uses the dielectric response (permittivity). All the three are merged to find the suitable atomic radii range from the polarisation energy.
Table 1. Required parameters for a microwave absorber.

| Symbol | Definition | Value |
|--------|-----------|-------|
| $R_L$  | Reflection Loss R.L | $-20$ dB |
| $f_r$  | RESONANCE FREQUENCY | $2.54$ GHz |
| $\Delta f_r$ | BANDWIDTH | $7.7$ GHz |
| $d$    | Thickness | $0.03$ m |
| $\zeta$ | Damping Factor | $1.5$ |
| $Q$    | Quality Factor | $0.33$ |

Table 2. Calculated atomic properties.

| Symbol | Definition | Value |
|--------|-----------|-------|
| $E_g$  | POLARISATION ENERGY LOWER LIMIT | $19.87$ eV |
| $E_g$  | POLARISATION ENERGY UPPER LIMIT | $3.22$ eV |
| $r_{\ell}$ | ATOMIC RADII LOWER LIMIT ($f_r = 2.54$ GHz) | $0.36$ Å |
| $r_{\alpha}$ | ATOMIC RADII UPPER LIMIT ANIONIC ($f_r = 2.54$ GHz) | $1.64$ Å |
| $r_{\alpha}$ | ATOMIC RADII UPPER LIMIT CATIONIC ($f_r = 2.54$ GHz) | $2.23$ Å |
| $r_{\alpha}$ | ATOMIC RADII UPPER LIMIT CATIONIC ($f_r = 10$ GHz) | $5.56$ Å |

Table 1 shows the desired parameters for a good microwave absorber [1–4]. The corresponding atomic parameters for such absorbers are then obtained in table 2 using the expressions and flowcharts in figures 1 and 2 based on [3, 4, 6–19]. Some intermediate parameters generated in the process are available in table 4.

2. Mathematical model

2.1. Required characteristics and parameters of a microwave absorber

As mentioned in table 1, the required characteristics of a microwave absorber are taken as per industrial and popular standards. The Reflection Loss is taken as $-20$ dB, giving 99 percent of absorption of incident wave. The input impedance of an absorber is always taken as higher than the free space impedance because of the higher dielectric permittivity and magnetic permeability of the absorber compound. The increased permittivity and permeability causes energy loss due to the dissipation of the absorbed radiation. The resonance frequencies are taken as $2.54$ GHz and $10$ GHz. The former is used for wireless communication while the latter is used for defence and military applications. The bandwidths are calculated using the Quality Factor of the absorber system. The Q factor is determined from the damping factor $\zeta$ which is taken as $\zeta < \approx (1/2)$ considering the absorber to be an overdamped system.

$$\zeta = \frac{1}{2Q}$$  \hspace{1cm} (1)

$$Q = \frac{2\pi f_r}{2\pi \Delta f_r} = \frac{\omega_r}{\Delta \omega_r}$$  \hspace{1cm} (2)

2.2. Resonance parameters of microwave absorbers

Reflection Loss of a microwave absorber is calculated using Transmission Line Theory. The incident medium for the absorber is free space. The reflection loss at the incident and absorber interface is given by following equation:

\[ R_{l} = 20 \log \left( \frac{Z_{in} - Z_{o, free}}{Z_{in} + Z_{o, free}} \right) \]  

where \( Z_{in} \) is the input impedance of the microwave absorber when modelled as a transmission line. \( Z_{o, free} \) is the characteristic impedance of the incident medium (free space) \([20, 21]\).

2.2.1. Input impedance and quality factor

Taking the Reflection loss to be -20 dB, which is a standard measure for 99 percent of absorption and the free space impedance as \( Z_{o} = 377 \text{ ohm (air)} \). Using the given values in equation (3), will get the following value of the input impedance.

\[ Z_{in} = 460.78 \Omega \]  

Ideally the characteristic impedance of an absorber should exactly match with the free space but due to practical limitations, it always varies from the ideal value. The deviated value of characteristic impedance of microwave absorber \( Z_{o, MA} \) can be found from the following equation. The given formula is based on maximum power transfer theorem and was used in reference [3] with respect to the shielding capability of iron ingredient based microwave absorbers.

\[ R.L. = 20 \log \left( \frac{Z_{o, MA}}{Z_{in} + Z_{o, MA}} \right) \]  

The input impedance of the microwave absorber can be written in terms of an Open circuit transmission line as given: [1]:

\[ Z_{in, MA} = Z_{o} \sqrt{\frac{\mu}{\varepsilon}} \tanh \left( \frac{-j2\pi \delta \sqrt{\mu\varepsilon}}{c} \right) \]  

### Table 3. Intermediate parameters used for evaluation.

| Symbol | Definition | Value |
|--------|------------|-------|
| \( Z_{in} \) | INPUT IMPEDANCE | 460.78 \( \Omega \) |
| \( Z_{o, MA} \) | CHARACTERISTIC IMPEDANCE | 184 \( \Omega \) |
| \( \mu_1 / \mu_2 \) | PERMEABILITY LOWER AND UPPER LIMIT | 1.35/4.4 |
| \( \varepsilon_1 / \varepsilon_2 \) | PERMITTIVITY LOWER AND UPPER LIMIT | 1.032/2.57 |
| \( n_1 \) | MIN REFRACTIVE INDEX | 1.6 |
| \( n_2 \) | MAX REFRACTIVE INDEX | 2.34 |
| \( k \) | WAVE PROPAGATION CONSTANT | \( 2.31 \times 10^{-10} \) |
| \( \alpha_p \) | POLARIZABILITY | \( 2.36 \times 10^{-28} \) |
| \( \eta_{air} \) | INTRINSIC IMPEDANCE | \( 2.9 \times 10^{-20} \) |
| \( \omega_p \) | DIPOLAR FREQUENCY | \( 2.4 \times 10^9 \text{ rad/sec} \) |
| \( \tau \) | TIME CONSTANT | \( 8.88 \times 10^{-12} \text{ sec} \) |
| \( \varepsilon^* \) | IMAGINARY PART OF PERMITTIVITY | \( 3.95 \times 10^{-3} \) |
The exponential decay factor $\alpha$, natural resonant frequency $\omega_n$, wave propagation constant $k$ and the time constant $\tau$ can be calculated from the Q factor of the absorber system with the following equations.

$$Q = \frac{\omega_n}{\tau} = \frac{1}{\tau\omega_n}$$  \hspace{1cm} (8)$$

$$\omega_n = \sqrt{\frac{k}{m}}$$  \hspace{1cm} (9)$$

Thickness ‘$d$’ of a dielectric based microwave absorber can be found using the following equation:

$$d = \frac{c}{4f_{r}\sqrt{\varepsilon_r}}$$  \hspace{1cm} (10)$$

Figure 1. Derivational flowchart for complete evaluation of microwave absorbers.
2.3. Lower limit of permittivity and permeability

Ratio of $\frac{\mu_r}{\varepsilon_r}$ is calculated using equation (3) with respect to a short circuit transmission line as shown below.

$$Z_d = \frac{Z_{in}}{Z_{ao}} = \frac{\mu_r}{\varepsilon_r}$$  \hspace{1cm} (11)

$$\frac{\mu_r}{\varepsilon_r} = 1.5$$  \hspace{1cm} (12)

Product of $\mu_r\varepsilon_r$ is calculated as follows considering the open circuit transmission line case.

$$Z_{oaMA} = Z_{oMA} \frac{\mu_r}{\varepsilon_r} \left( \frac{2\pi d \sqrt{\mu_r \varepsilon_r}}{c} \right)$$  \hspace{1cm} (13)

$$\mu_r \varepsilon_r = 1.6$$  \hspace{1cm} (14)

From the above equations individual values of permeability and permittivity is calculated giving $\varepsilon_r = 1.032$, $\mu = 1.55$.

2.4. Polarizability and related parameters

The polarizability of a material can be calculated in terms of natural resonance frequency, operational resonance frequency, damping constant as shown below [4]:-

$$\alpha_p = \frac{c^2m(\omega_0^2 - \omega^2)}{m^2(\omega_0^2 - \omega^2)^2 + 4\eta\omega^2} - \frac{2c^2\eta\omega}{m^2(\omega_0^2 - \omega^2)^2 + 4\eta\omega^2}$$  \hspace{1cm} (15)

The damping constant can be determined from the wave propagation constant $k$ and the mass of electron $m$, as given by:-
This is the Clausius-Mosotti equation which relates the relative permittivity to the number of dipoles per unit given by

\[ \epsilon = 1 + \frac{n_o^2}{n_u^2} \]

2.4.2. Complex permittivity and conductivity

Complex Permittivity is an important electrical property of absorbing materials. It depends on resonance frequency, bandwidth, time constant as per given mathematical equations [10].

\[ \epsilon_\omega = \epsilon'_\omega + \epsilon''_\omega \]

\[ \epsilon'_\omega = \chi'_\omega + 1 = \frac{\omega^2 - \omega^2}{(\omega^2 - \omega^2)^2 + \frac{\omega^2}{\tau^2}} + 1 \]

\[ \epsilon''_\omega = \frac{\omega^2}{(\omega^2 - \omega^2)^2 + \frac{\omega^2}{\tau^2}} \]
Here, the value of $\omega_p$ is given as

$$\omega_p^2 = \frac{n_1 q^2}{\varepsilon_0 m}$$

where $n_1$ is the total number of dipoles per unit volume given by $N$ as calculated in equation (18), $m$ is the mass of electron. Solving above equation, the natural dipolar resonant frequency $\omega_p$ can be calculated.

Conductivity of the absorber can be calculated from $\sigma = \frac{\sigma}{\omega \varepsilon_0}$

2.5. Upper limit of permeability and permittivity

Based on the below equation as

$$\varepsilon'' = \frac{na_p \varepsilon}{2\pi \nu}$$

where $a_p = 0.1$ gives the power absorption coefficient, and $n$ is the refractive index given by $n = \sqrt{\mu}$, $\nu$ is the working frequency, $\varepsilon''$ is the imaginary part of permittivity as calculated in equation (21). Evaluating the equation (23), the upper limit of the refractive index $n_u$ is given by:

$$n_u = \sqrt{\mu} = 2.1$$

Using cauchy’s dispersion equations, the distortion effects at higher refractive index can be accounted to give the final value of the refractive index as $n_2$: The electronic susceptibility can be given as:

$$\chi_e' = \frac{\omega_p}{\omega_0}$$

The different constants for relating susceptibility to refractive index are:

$$A = 1 + \chi_e(0) = n_u^2$$

$$\omega_0^2 = \omega_p^2$$

$$B = (2\pi \nu)^2 \frac{\chi_e(0)}{\omega_0^2}$$

$$C = \frac{B}{2A^{1/2}}$$

$$n_2 = n_u + \frac{C}{\lambda_0}$$

The upper value of permeability can be calculated from the absorption equation for magnetic based microwave absorber as given below, where $d_m$ represents the thickness of a magnetic microwave absorber, $(SE)_a = 0.99$ is the absorbed power.

$$d_m = \frac{1}{4} \left( \frac{c}{f_m \sqrt{\mu \pi \sigma}} \right)$$

$$d_m = 0.0233$$

$$(SE)_a = 8.7d_m \sqrt{f_m \pi \mu \sigma}$$

$$\mu_r = 2.57$$

2.6. Polarization energy, global hardness factor and theoretical radii

2.7. Polarization energy

Below is the equation of the molar fraction of oxides [15]

$$R_m = \left( \frac{n^2 - 1}{n^2 + 2} \right) V_m$$

$n$ is the linear refractive index, $V_m$ is the molar volume.

The polarizability can be related to the molar refraction ratio as given below:

$$\alpha_m = \frac{3}{4\pi N_A} R_M$$

$\alpha_m$ is the polarizability as given in (15),

$N_A$ is the avagadro number.
The relation between the energy gap of the oxide and the molar refraction ratio is given by:

\[ E_G = 20 \left(1 - \frac{R_m}{V_m}\right)^2 \]  

(37)

Here, an important concept of metallization criteria \((M)\) should be considered which acts as a threshold for the possibility of the formation of the solid soluble compounds, it is given by:

\[ M = 1 - \frac{R_m}{V_m} \]  

(38)

Using equation (35), (37), (38) the polarization energy of the absorber compound can be found. The given energy value is then used in the below equation to calculate the corresponding atomic radii value. Both the lower and the upper atomic radii limit can be calculated by keeping the respective refractive index value in equations (35), (37).

\[ R = \left[ \frac{q^2}{2} \frac{(eV)}{\eta} \right] \frac{1}{\eta} \]  

(39)

2.7.1. R corresponding to lower limit
Keeping the value, the atomic radii are:

\[ R = 0.36 \, \text{Å} \]  

(40)

\[ E_G = 19.87 \, eV \]  

(41)

2.8. R corresponding to upper limit: anionic

\[ E_G = 4.34 \, eV \]  

(42)

\[ R = 1.64 \, \text{Å} \]  

(43)

2.9. R corresponding to upper limit: cationic

Radius value corresponding to the upper refractive index limit as given in equation (26)

\[ n = 2.34 \]  

(44)

\[ R = 2.23 \, \text{Å} \]  

(45)

2.10. Effective energy parameter

From the derived range of atomic radii, suitable material compositions can be found out by formulating a way of comparing the compatibility of different elements towards each other based on their effective energy parameter \(P_e\) [19]. This Parameter serves as a measure of the element’s tendency to ionize. The parameter depends on the effective charge of nucleus, effective quantum number, global hardness factor and atomic radii. Figure 2(a) depicts the calculation of the effective energy parameter for the individual elements [14, 17–19]. Table 2 enlists the polarization parameters used for modelling the absorber. This parameter is the ratio of spatial energy parameter to the atomic radii. The effective quantum number was calculated from the sum of individual atomic orbital exponents of the element divided by the their respective atomic number [17]. For any compound, the effective energy parameter is used to calculate the balance between the polarisation tendencies of the cations and the anion. If it is comparable, the compound will be suitable for Microwave Absorption at desired frequency and bandwidth. Using the effective energy parameter balancing equations are formed to predict the material compositions of microwave absorbers. The materials considered here are oxides and ferrites. Flowchart 2 shows all the equations and formulae involved in calculating the effective energy parameter. The given parameters are calculated for the entire elements from atomic number one to eighty providing a dataset (table 7) to pick and select elements for our microwave absorber based on their polarization efficiencies. The general formula of spatial energy parameter is [19]

\[ \frac{1}{q^2} + \frac{1}{\eta} = \frac{1}{P_e} \]  

(46)

\(r_i\) is the atom orbital radius, \(\eta\) is the global hardness factor, Considering the polarization energy equivalent to the Global hardness factor, which is none other than the ability of a chemical species to form bond with its neighbouring atom/molecule, as given by :-
The effective energy parameter for all the elements of the periodic table starting from Hydrogen to Gold is tabulated in Table 7. The table forms an important database in analysing the suitability of various compounds as microwave absorbers, which is discussed in coming sections. Python code has been used to do the calculations for the effective quantum number and the parameters of Table 7. The python script along with the input and output files can be found in Supplementary Information.

### 2.11. Magnetic microwave absorbers

Magnetic losses are an important part of the wave absorption phenomenon in magnetic material based microwave absorbers. Similar to the electric dipoles in dielectric MA, magnetic dipole moments of the constitutive elements affect the overall absorption. There are two types of magnetic dipole moment, spin and orbital angular moment. The former is associated to the real part of permeability and the latter to the imaginary part \[22, 23\]. In d-shell compounds like ferrites the former is dominant because of quenched orbital momentum.
being tied to the easy magnetization direction (EMD), while in the f-shell compounds the latter is dominant owing to the asymmetrical orbitals [24, 25]. The flowchart 2(b), shows the steps to calculate suitable range of magnetic dipole moments for the given absorber specifications.

In order to calculate the range of magnetic moments for d-shell and f-shell elements, suitable for microwave absorption application, permeability value will be taken in consideration. For d-shell, the desired frequency and thickness of the microwave absorber will give the imaginary part of the permeability, which is further used to calculate the volume, atomic susceptibility and the spin magnetic moment. For the f-shell, the real part of the permittivity gives the overall susceptibility which is further used to obtain the orbital angular momentum as shown in the flow chart. Along with the calculated range, the selection of suitable value of magnetic dipole moment also depends on the difference in the cationic and the anionic polarisation energy of the compound [26]. table 6 and shows the various magnetic parameters with their definitions. tables 8 and 9 tabulates the calculated values of the magnetic parameters for d and f-shell elements respectively.

The spin dipole moment for the d-shell elements can be calculated as:

$$\mu_s = 2.84 \sqrt{\chi_A T} B.M$$

In the above equation $\chi_A$ is the atomic susceptibility, B.M is the bohr magneton in C.G.S units

$$\mu_{B} = 9.27 \times 10^{-21} \text{erg/gauss.}$$

For the f-shell elements, considering the skin depth and the conductivity due to the associated orbital angular momentum, the dissipative factor of permeability can be calculated as [27]:

$$\mu'' = \frac{2\pi \mu_s (\mu' \gamma \sigma)^2 f}{3}$$

With the skin depth given as:

$$\delta = (f\pi \sigma \mu)^{1/2}$$

Table 9 shows upper and lower calculated values of the spin dipole moment along with the above magnetic parameters for f-shell elements for respective permeability values. In the above equations, the former one gives the orbital dipole moment, while the latter one gives the spin dipole moment.

The imaginary part of permeability, for the d-shell elements, can be calculated as follows:-

$$\mu'' = \frac{c}{2\pi df_m}$$

The atomic susceptibility can be calculated by the product of molar volume $V_M$ and Avagadro constant $N. For f-shell $\mu_T = \mu_f$, which is given below:-

$$\mu_f = \frac{1}{\mu_B} \sqrt{\frac{\chi_m (kT)}{n_l \mu_s}}$$

In above equation, $\chi_m$ is the susceptibility, k is the boltzmann constant with value $k = 1.38 \times 10^{-23}$, $n_l$ is the total number of magnetic sites or the number of atoms per unit volume. But a discrepancy occurs at magnetic resonance, which is the condition of maximum absorption, leading to the splitting of the energy spectrum of the outer d-orbital, the splitting occurs from one atom to a maximum of N atoms, integrating of the splitting level, gives $n_l = N^2$. table 8 shows the orbital dipole moment and other magnetic parameter for d-shell elements [26].
3. Selection criteria

Figure 4 shows the application of the given model on experimentally verified compound. The range of the upper and lower atomic radii serves as a criteria for material selection. It gives a broad idea of the suitability of different elements in the compound for a specified frequency. The derived radius values can be used to choose the cation and the anion required for the microwave absorber by matching their atomic radii to the derived values.

Table 7. Atomic and polarisation parameters for all elements.

| Element | \( n \) | \( \rho \) | \( \sigma \) | \( q \) | \( p_{\gamma}(\text{MeV}) \) | \( p_{\gamma}(\text{F}) \) |
|---------|-------|-------|-------|-------|-----------------|-----------------|
| He      | 0.8   | 0.502 | 1     | 3     | 2.672           | 0.422           |
| Li      | 1.1   | 0.622 | 0.58  | 2     | 2.347           | 4.016           |
| Be      | 1.2   | 0.605 | 0.97  | 3     | 3.217           | 4.246           |
| B       | 1.9   | 0.814 | 1.3   | 2     | 2.709           | 8.832           |
| C       | 2.0   | 0.853 | 1.825 | 3     | 3.117           | 11.047          |
| N       | 2.0   | 0.542 | 1.95  | 3     | 3.861           | 13.23            |
| O       | 2.0   | 0.463 | 2.75  | 3     | 4.505           | 13.574          |
| F       | 2.0   | 0.801 | 2.4   | 3     | 5.148           | 17.693           |

Note.
<sup>a</sup> Effective Principal Quantum Number.
<sup>b</sup> Taken from [14].

Yellow rows shows elements compatible for 2.54 GHz Band and Green rows shows elements compatible for both 2.54 GHz and 8 GHz Band.

3. Selection criteria

Figure 4 shows the application of the given model on experimentally verified compound. The range of the upper and lower atomic radii serves as a criteria for material selection. It gives a broad idea of the suitability of different elements in the compound for a specified frequency. The derived radius values can be used to choose the cation and the anion required for the microwave absorber by matching their atomic radii to the derived values.
fulfilling the above criteria the selected materials are then compared for compatibility, based on the matching of the polarisation abilities using the balancing equation. Tables 10 and 11 provide the constant parameters used for the formulations and the balancing equations respectively. For predicting a compound based on the proposed model, the following steps should be taken:

- First step is to select the elements from the calculated atomic radii range. The element should be between the derived upper and the lower atomic radius.
- The selected elements will serve as cations against oxygen as anion in oxide compounds. The compound structure can be either of a pervoskite or a ferrite.
- After selecting the elements, the elements should then be compared based on their effective energy parameter. Using the values of $P_E$ from table 7, the compound should satisfy the balancing equations given in table 11. Either of the two equations can be used depending on if the compound is dielectric or magnetic.
- Next step is as shown in figure 3, which provides an empirical method for calculating the compositional parameters for the predicted absorber. In case of mixed cations, the molar ratio of cation can be found by taking two cations at a time. Taking two cations $a$ and $b$ (with cation a radius larger than b) the molar ratio of cation a is given by:

$$M_a = \frac{r_a \times P_{Ea}}{r_b \times P_{Eb}}$$

and for cation b it is given by $C_b = 1 - C_a$. If there are more than two cations involved, cation a, b, c(with

| Table 8. Magnetic parameters d-shell. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| $\mu$ | $\mu^d$ | $\delta$ | $\chi_m = \mu - 1$ | $\mu_1 = \frac{1}{P_1} \frac{2\sin(\delta)}{\delta N_{\text{orbbal}}}$ |
| 1.032 | 269 | 3.4 | 0.032 | 9.4 |
| 2.57 | 20.59 | 2.34 | 1.57 | 2.53 |

| Table 9. Magnetic parameters f-shell. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| $n$ | $f_m$ | $\mu_E$ | $\chi_{\text{atomic ratio}}$ | $\chi_{\text{magnetic dipole moment}}$ |
| 1.6 | 2.54 GHz | 1.0192 | 1.53X10^2 | $2.32 \times 10^{-5}$ |
| 2.1 | 7.7 GHz | 1.3377 | $2.69 \times 10^{-2}$ | $4.08 \times 10^{-2}$ |

| Table 10. Notations used in figure 3. |
|-----------------|-----------------|-----------------|-----------------|
| $ABo_3$ | Pervoskite Structure with A,B cation and Oxygen as anion |
| $P_{Ea}$, $P_{Eb}$, $P_{Ec}$ | Effective energy parameter for cation A,B,C as calculated in table 5 |
| $M_a$, $M_b$, $M_c$ | Respective molar ratio of each cation in the compound |
| $r_{a}$, $r_{b}$, $r_{c}$ | Intermediate molar ratio value in three cation based compound |

| Table 11. Balancing equations for dielectric and magnetic compounds. |
|-----------------|-----------------|-----------------|-----------------|
| Balancing equation | Dielectric | $P_{E1} = \sum_{\text{cations}} P_{E} \times \text{atomic ratio} \times \text{valency}$, $P_{E2} = \frac{P_{\text{atomic ratio}}}{\text{valency}} \times \text{no of atoms}$ |
| Magnetic | $P_{E1} \times N_{\text{orbs}} \times \text{Number of electrons in O} \times Z(\text{Atomic Number of O})$ |

$$P_{E1} = \sum_{\text{magnetic dipole moment}} \times n \times \text{valency}$$
Figure 3. Flowchart for atomic/molar ratio calculation.

Figure 4. Procedure to analyse a compound for its suitability as microwave absorber: LaMnO$_3$. 

| Cations | Anions |
|---------|--------|
| Elements | La | Mn | O |
| $P_R$ | 0.4221 | 1.2423 | 18.0567 |
| Atomic ratio | 1 | 1 | 3 |
| Valency | +3 | +2 | -2 |

Using Balancing equation for dielectric:

$$\Delta P_R = \frac{P_{R1} - P_{R2}}{P_{R1}}$$

Dipole moment of Mn

$$= 5.82, N_e=8, Z=8$$

$$= 3.75 - 3.1$$

X X X = 5.82X2
atomic radii \( a > b > c \) then cation \( b \) and \( c \) can be grouped together and evaluate the above equation for cation \( a \) and \( b \) then for cation \( b \) and \( c \) separately so that with molar ratio of cation \( a \) as \( \text{Ca} \), for \( b = \frac{\text{MM}}{r_{P}} \)

\[ M_b = M_{b_i} \times \frac{r_{b_i} \times P_{I_i}}{r_i \times P_{I_i}} \]

\[ M_c = M_{b_i} - M_b \]

4. Result

The computational methodology explained above was verified by applying it on experimentally certified microwave absorbing compounds given in Table 12. Based on this some new compounds are also proposed in table 13 as potential microwave absorbers for further study. The compounds analysed here are oxides, in pervoskite and ferrites structures. Oxygen forms the anionic part whereas the cations can be mixed or single along with magnetic elements.

5. Conclusion and future work

The theoretical model presented here gives an approach to predict the material composition for absorption applications. The method when applied to proven compositions gives an insight into their atomic level behaviours. Microwave absorption is cumulative effect of different physical phenomenon which are related to each other via energy conversion and dissipation. The idea suggested here will help in bringing out this complex relationship of the electrical, magnetic and atomic parameters and can benefit in forming new compositions. The compositions for multiple cations and anions can be predicted using the work here, which will enable formation of new, chemically stable, superior physical properties based absorbers. The proposed approach is likely to improve the success rate of the experimental procedures for making new compounds for varied absorber application. It is also helpful in understanding the relation between the characteristic properties of an absorber with the fundamental and atomic properties of the constitutive element breaking the complex parameters to a set of known fundamental parameters. The work can further be improvised by adding other constraints based on the geometrical structure of the compound and effect of material doping, ion displacements in the composition. The given model can also serve as a platform for making AI (Artificial Intelligence) and ML (Machine Learning) based algorithms for automating the process of material selection.
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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix

The calculation for the effective quantum number and table 7 is done using python script. The input and output data is in excel workbook as input.xlsx and output.xlsx respectively. The python script is written using Microsoft Visual Studio. The files are provided as supplementary files.

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