Theoritically determine a predictive model for a Microwave Absorber using physical ,electrical, magnetic and atomic properties of constitutive elements

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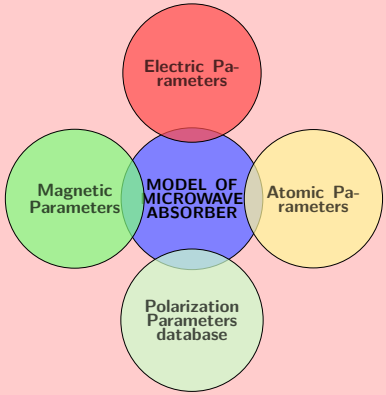
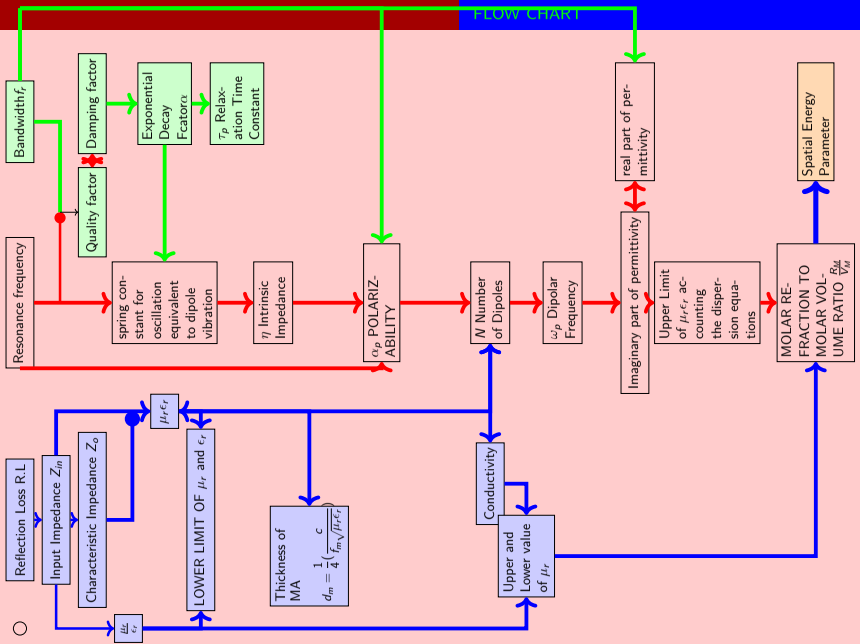
OBJECTIVE

- **THEORITICAL MODEL** MICROWAVE ABSORBERS are key highlights in today's 5G era. There has been lots of theoritical study on the topic but all are mainly restricted to the bulk electrical properties.
- With this work, we intend to develop a model that will include not only the electrical properties , but also will have an **insight into the atomic and fundamental properties of matter** that will affect the performance of MA.
- **This model can be used as a basis to select suitable material for a specific application before the experimental trials**
- **Can be used in transferring experimental process to industrial level Production.**
- **Database of all elemenets with their atomic and spatial polarization energy parameter.**
- **Provides more logical and mathematical approach towards the designing of MA.**
- **New materials with excellent mechanical properties and high absorption can be engineered**




Bandwidth f_r
Damping factor
Exponential Decay Fcator α
τ_p Relaxation Time Constant
Quality factor
real part of permittivity
Spatial Energy Parameter
Resonance frequency
spring constant for oscillation equivalent to dipole vibration
η Intrinsic Impedance
α_p POLARIZABILITY
N Number of Dipoles
ω_p Dipolar Frequency
Imaginary part of permittivity
Upper Limit of $\mu_r\epsilon_r$ accounting the dispersion equations
MOLAR REFRACTION TO MOLAR VOLUME RATIO $\frac{P_M}{V_M}$
$\mu_r\epsilon_r$
Reflection Loss R.L
Input Impedance Z_{in}
Characteristic Impedance Z_o
$\frac{\mu_r}{\epsilon_r}$
LOWER LIMIT OF μ_r and ϵ_r
Thickness of MA $d_m = \frac{1}{4}\left(\frac{c}{f_m\sqrt{\mu_r\epsilon_r}}\right)$
Conductivity
Upper and Lower value of μ_r

THEORITICAL PREDICTIVE MODEL

IMPEDANCE MATCHING

For the EMI shielding applications, the prerequisite is to minimize the reflection and maximize the absorption of the incident EM wave.Keeping the Relection Loss value to be R.L = -20 dB, which means that 99percenatge of microwave is absorbed, the input impedance *Zin* at the air–material interface can be calculated as:-

$$RL(dB) = 20log \mid \frac{Z_{in} - Z_o}{Z_{in} + Z_o} \mid \quad (1)$$

Using the above , we can evaluate the characteristic impedance of the microwave absorber , which is related to the intrinsic parameters of the material:-

Cont.

1. **Input Impedance** Keeping the standard value of reflection loss of -20 dB , and air impedance of $Z_o = 377\Omega$,we get $\boxed{Z_{in} = 377\Omega}$.
2. **$Z_o m$ of MA** using the value of above input impedance of MA , we can get the characteristic impedance of the $\boxed{R.L = 20\log(\frac{Z_o}{4Z_{in}}) \text{ and } Z_o = 184\Omega}$.
3. **Qulaity factor Damping Constant** Considering the system to be overdamped, taking the resonance and bandwidth frequency we get $Q = \dfrac{2\pi(f_r)}{2\pi\Delta(f_r)}$ and $Q = 0.33, \zeta = 1.5$.
4. **exponential decay factor α** From Q and ω_o, we can get $\boxed{Q = \frac{\alpha}{\omega_0} \text{ and } \alpha = 2.39X10^{10}}$

Cont.

5. **RATIO OF RELATIVE PERMEABILITY TO PERMITTIVITY** The equation is given by $R_L = 20log_{10}\left|\frac{\sqrt{\frac{\mu_r}{\epsilon_r}}-1}{\sqrt{\frac{\mu_r}{\epsilon_r}}+1}\right|$,using this we can get $\boxed{\frac{\mu_r}{\epsilon_r} = 1.5}$

6. **PRODUCT OF RELATIVE PERMEABILITY TO PERMITTIVITY** The product can be found by

$$Z_{in} = Z_{om}\sqrt{\frac{\mu_r}{\epsilon_r}}\left(\frac{2\pi\nu d\sqrt{\mu_r\epsilon_r}}{c}\right)$$

, using the above values we get where $\boxed{\mu_r\epsilon_r = 1.6}$ and further solving we get $\boxed{\mu_r = 1.55 and \epsilon_r = 1.032 \text{ Lower Limit of Permeability and Permeability}}$.

Cont.

7. **Spring Constant of Dipoles and Intrinsic Impedance** Both of the value can be found by $k = {\omega_o}^2 * m$ and $\eta = 2\sqrt{km}$, substituting values we get $\boxed{k = 2.31X10^{-10} \text{ and } \eta = 2.36X10^{-28}}$. This can be explained by considering the osciltaions of dipoles , created by the incident microwaves ,to be equivalent to the mass spring system.
8. **POLARIZABILITY α_p** Using the above values we can get the polarizability as

$$\alpha_p = \frac{e^2 m({\omega_o}^2 - \omega^2)}{m^2({\omega_o}^2 - \omega^2)^2 + 4\eta\omega^2} - \frac{2e^2\eta\omega}{m^2({\omega_o}^2 - \omega^2)^2 + 4\eta\omega^2}$$

and the value as $\alpha_p = 2.36X10^{-28}$ or $\alpha_p = 236\text{Å}$.

Cont.

9. **NUMBER OF DIPOLES** The polarizability is used in CLAUSSIUS MOSOTTI equation to calculte the Number of dipoles N_d ,given by

$$\frac{(\mu\epsilon)-1}{(\mu\epsilon)+2}=\frac{N\alpha_p}{3\epsilon_o}$$

,giving $\boxed{N_d = 1.87X10^{16}}$

10. **DIPOLAR RESONANT FREQUENCY** The above value can be used to calculate the Dipolar resonant frequency ,which is the ideal frequency for all the dipoles to be in resonance.$\omega_p^2=\frac{n_e q^2}{\epsilon_o m}$, at the same time calculating the time constant $\tau=\frac{1}{\zeta\omega_o}=8.88X10^{-12}sec$, giving values $\boxed{\omega_p = 2.4X10^9 rad/sec \text{ and } \tau = 8.88X10^{-12}sec}$.

Cont.

11. COMPLEX PERMITTIVITY and CONDUCTIVITY The real and imaginary part of permittivity can be calculated by below equations

$$\epsilon_r^{'} = \left(\frac{\omega_P^2(\omega_o^2 - \omega^2)}{(\omega_o^2 - \omega^2)^2 + \frac{\omega^2}{\tau^2}}\right) + 1$$

and

$$\epsilon_r^{''} = \frac{\omega_P^2(\frac{\omega}{\tau})}{(\omega_o^2 - \omega^2)^2 + \frac{\omega^2}{\tau^2}}$$

,the real part is equal to unity as calculted earlier with lower data points,

$\epsilon^{''} = 3.95X10^{-3}$ substituting this in $\epsilon_r^{''} = \frac{\sigma}{\omega\epsilon_o}$, we get $\sigma = 5.29X10^{-4} siemens$

Cont.

12. **UPPER LIMIT OF PERMEABILITY AND PERMITTIVITY** Using the value of power absorption coefficient $a_p = 0.1$ and ϵ'' , higher value of n can be calculated as $\epsilon_r'' = \frac{na_pc}{2\pi\nu}$ with value $n = 2.1$.Using the cauchy's dispersion equation to compensate for the distortion due to higher cationic size we get $n = 2.34$
13. **MAXIMUM VALUE of PERMEABILITY** With $(SE)_A = 8.7d\sqrt{f_o\pi\sigma\mu}$, maximum value of $\mu_r = 4.4$ can be obtained which is further used in the magnetic dipole moment calculation as discussed later.
14. **POLARISATION ENERGY** The value of the set of refractive indices to calculate the energy involved in the polarization as $R_m = (\frac{n^2{}_o - 1}{n^2{}_o + 2})V_m$ laeding to $E_g = 20(1 - \frac{R_m}{V_m})^2$, here R_m is the molar fraction of oxide and V_m molar volume . With E_g being equivalent to the global hardness factor η , the theoritical radii set can be obtained corresponding to the two limits as $R = 0.36$Å and $R = 2.23$Å.

Cont.

15. ATOMIC PARAMETER DATABASE Further using the values of effective principal quantum number, effective nucleus charge, orbital exponent, global hardness factor , a table is created for all elements calculating their effective spatial energy parameter which can be compared to the polarization enrgy obtained in above equation to check the suitability of different elements for Microwave Absorber Applicayions. These parameter can also be applied to different compositions in such a way to balance the overall charge energy balance of both cationic and anionic side as shown later.

ATOMIC PARAMETERS

The polarisation Energy will be calculated using the principle of adding inverse values of volume energies and kinetic parameters whcih has been used in many different physical and chemical processes. Since Polarisation can be related to the force exerted by the valence electrons that is the electron affinity,and their inertness to form direct bond that is the ionization potential, screened through nucleus charges,it can be calculated proportionally via the inverse addition of orbital energy (accounting for the attraction or repulsion by electrons) and the effective nucleus energy.

$$\frac{1}{q^2} + \frac{1}{\eta} = \frac{1}{P_o}$$

where η is the global hardness factor $q = \frac{z^*}{n^*}$, z^* is the effective charge of nucleus and n^* is the effective main quantum number. $P_o(eV\text{Å})$ is called the spatial energy parameter and $P_E(eV\text{Å})$ is called the effective P-parameter for polarization. P_E is a physical parameter , accounting for the averaged polarisation energy over the valence electrons. η is the global hardness factor , which is calculated from the ionization potential and the electron affinity of the atom. By considering the simple electrostatic coulumbic forces across atoms,it can also be calculated as $\eta = \frac{e^2}{2R}$.

Effective principal quantum number can be calculated as a cumulative effect of the orbiatl exponent value ξ of each shell occupied, the outer shell value and the average spin of the outer shell.

Effective principal quantum number = orbital exponents of each shell (taking effect of screening charges)

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outer shell Orbital exponent*outer shell quantum number*average spin

Similarlt the effective nucleus charge $q(eV\text{Å})$, can be calculated from the nucleus charge minus the screening effect.

The last parmeter that is P_E can be calculated as

$$P_E = \frac{P_o}{r_i}$$

,where r_i(Å) is the atomic radii of atom. The effective polaristaion parameter can be used for comparing the suitability of different elements in different material compositions for the Microwave Absorbing Applications. [Vineeta Shukla. Review of electromagnetic interference shielding materials fabricated by iron ingredients.

MATERIALS

- METALLIC PERVOSKITE MATERIAL Benefits of using pervoskite is broad EM wave absorption spectrum, environment stability, chemically inert,unique physical properties for metallic ground states,balance between permittivity and peremability[?].
- Pervoskite materials have already been established as a microwave dielectric used in wireless communication devices viz. resonators,filters, temperature stable capacitor as shown in figure.
- These materials , which have been studied for more than a half century, shows immense potential as microwave absorbers owing to its resonating dielectric polarization across its cryatal structure Some examples include$LaNiO_3$,.
- HIGH ENTROPY OXIDES HEOs are new engineered materials that have a multi cationic configuration , leading up to an increase in the entropy of the compound. The entropy stabalization imparts them functional properties(more stable dielectric behaviour).These properties can be engineered with much flexibility. Examples are $(Co_{0.2}Cu_{0.2}Mg_{0.2}Ni_{0.2}Zn_{0.2})O_3$ [24]

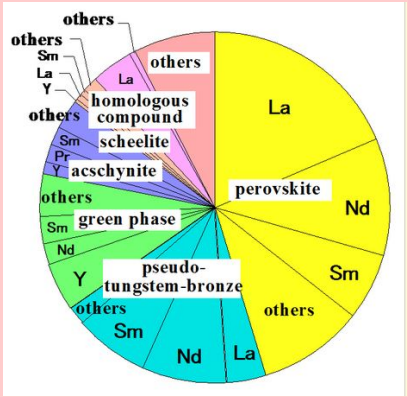


Figure: microwave dielectrics [22]

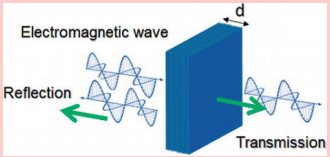
MATERIALS

- FERRITES Ferrites have found popularity as Microwave Absorbers owing to the magnetic losses along with dielctric losses giving high absorption at wide frequency range.Impedance matching of Ferrite is more improved than pure dielectrics because of low eddy current loss[16].
- X-type HEXAGONAL FERRITES, with high saturation magnetization, low coercivity, excellent chemical stability serve as good microwave absorbers.
- RARE EARTH elements have certain relaxation properties which enhances the EM wave properties of ferrites[23].
- MANGANITE MATERIALS manganites like $La_{0.8}Ca_{0.2-x}Ag_xMnO_3$ (x=0.05 to 0.15) have shown good microwave absorption propeties as shown in [20, 16]
- RARE EARTH doped OXIDES rare earth doped oxides have shown better microwave absorption properties with wide peak behaviour. The dynamic behaviour of compound changes with rare earth doping [17]

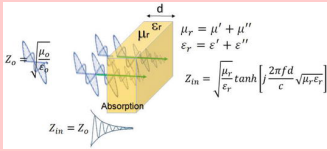
MAGNETIC PARAMETERS

S.No	d-shell	f-shell
Real Part of Permeability	$\mu^{'}$	$\mu^{'}$
Imaginary part of Permeability	$\mu^{''} = \frac{c}{2\pi d f_m}$	$\mu^{''} = \frac{2\pi\mu_o(\mu^{'})^2\sigma\delta^2 f}{3}$
Suscpetibility	Atomic Susceptibilty χ_A	Molar Susceptibilty χ_M
Magnetic Dipole Moment	Spin Magnetic Dipole Moment $\mu_s = 2.84\sqrt{\chi_A T}B.M$	Orbital angular moment $\mu_J = [\frac{3kT\chi_A}{N{\mu_B}^2}]^{1/2}$

MICROWAVE ABSORBERS



(a) LAYOUT OF MA



(b) ELECTRICAL PARAMETERS OF MA

PERMITTIVITY AND PERMEABILITY

$$\epsilon = \epsilon^{'} + \epsilon^{''} \tag{2}$$

The real part => measure of amount of energy stored in the material due to external electric field. The imaginary part => measure of dissipation of electrical energy.

$$\mu = \mu^{'} + \mu^{''} \tag{3}$$

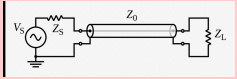
The real part => measure of amount of energy stored in the material due to external magnetic field. The imaginary part => measure of dissipation of magnetic energy.

LITERATURE REVIEW

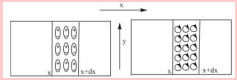
reference	Work
[Ying Liu, Rui Tai, Michael GB Drew, and Yue Liu. Several theoretical perspectives of ferrite-based materials—part 1: transmission line theory and microwave absorption. *Journal of Superconductivity and Novel Magnetism*, 30(9):2489–2504, 2017]	Transmission Line Theory was used to model the ferrite base and find a relationship between the elctric and magnetic stru material to the microwave absorption. The work also shows of Transmission Line Theory to the band theory of solids
([B.R.K Gupta Jai Shankar, H.P. Sharma. Electronic polarizabilities of ions in transition metal oxides. *Solid State Communications*, 21(4):359–361, 1977])	Evaluation of Electronic Polarizability of tranistion metals fr spective ionic radii.The changes in the ionic state of a transit used to mathematically calculte the polarizabilities
[Robert D Shannon and Reinhard X Fischer. Empirical electronic polarizabilities in oxides, hydroxides, oxyfluorides, and oxychlorides. *Physical Review B*, 73(23):235111, 2006]	The mean total polarizabilities of oxides,hydroxides,oxyfluorid prically calculated from the free cation polarizabilities . Ther cation of polarizability additive rule and least square procedure the cation coordination
[MN Azlan, MK Halimah, SZ Shafinas, and WM Daud. Polarizability and optical basicity of er3+ ions doped tellurite based glasses.	Lorentz-Lorenz equation was used to theoritically calculate electronic and oxide ion polarizability of oxide glasses . T metallization criteria was observed on the refractive index

MICROWAVE ABSORBER THEORY AND PHENOMENON

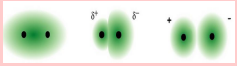
The existing Transmission Line Theory , which is used to analyse the microwave circuits is now being used by material scientists to evaluate different materials used as microwave absorbers.



(a) Transmission Line Schematic



(b) Electrical and Magnetic dipolar moments[21]



(c) Deformation due to polarization[18]

In some of the microwave absorbers , especially composite or dispersive materix based , there is MAXWELL-WAGNER POLARIZATION or space charge polarization ,induced by an electrical potential resulting from internal charge builds at the interfaces in a heterogenous material[**?**]

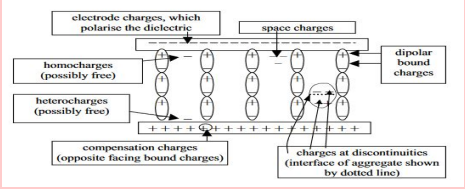


Figure: DIFFERENT TYPES OF POLARIZATIONS[14]

TRANSMISSION LINE THEORY

- USE OF TRANSMISSION LINE THEORY to theoritically model the resonant and non-resonant oscillation based microwave absorption.
- This theory , establishes the interaction of net absorption to the physical electric and magnetic parameters of the MA. The above model is independent of underlying absorption mechanism viz. as absorption from resonance, dielectric or magnetic media , from resonance or forced non resonance oscillation.
- GENERAL PREDICTIVE MODEL which can be used to understand the behaviour
- THis theory can be used to find the influence of a variety of physical parameters and material properties arising from the atomic configurations, on their microwave absorbing characteristics.
- This theory provides a way of deeper undersatnding into the required materislistic aspects of an ideal MA , which can lay a platform to design and explore new engineered materials for various applications

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