Lecture 11, Part 1: Glass dielectrics for microelectronics and energy applications - Dielectric properties and metamaterials

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Dielectric Properties and Metamaterials

Mike Lanagan
Materials Research Institute
Penn State University

US-Japan Winter School on New Functionality in Glass
January 15, 2008
Kyoto Japan
Dielectric Properties and Metamaterials

• Dielectric Properties (i.e. Permittivity)
  – Fundamental frequency dependence

• Metamaterials
  – Negative permittivity and refractive index
  – Based on resonance response
  – Discussion on the potential of glass as a meta-material
Electromechanical effects (piezoelectricity)

Electrothermal Effects (pyroelectricity)

Thermoelastic effects

ELECTRICAL

THERMAL

MECHANICAL

Properties studied so far at Winter School
Properties studied so far at Winter School
Dielectric Polarization

• Contributes to Permittivity
• 4 basic mechanisms
  – Electronic
  – Ionic
  – Rotational or Dipolar
  – Space charge
External Electric Field Polarizes a Material

Polarization charge density on the surface of a polarized medium is related to the normal component of the polarization vector.

Relative Permittivity and Polarizability

\[ \varepsilon_r = 1 + \frac{N\alpha_e}{\varepsilon_o} \]

\( \varepsilon_r \) = relative permittivity

\( N \) = number of molecules per unit volume

\( \alpha_e \) = electronic polarizability

\( \varepsilon_o \) = permittivity of free space

Assumption: Only electronic polarization is present

(a) Valence electrons in covalent bonds in the absence of an applied field.

(b) When an electric field is applied to a covalent solid, the valence electrons in the covalent bonds are shifted very easily with respect to the positive ionic cores. The whole solid becomes polarized due to the collective shift in the negative charge distribution of the valence electrons.
(a) A NaCl chain in the NaCl crystal without an applied field. Average or net dipole moment per ion is zero.

(b) In the presence of an applied field the ions become slightly displaced which leads to a net average dipole moment per ion.
Rotational or Dipolar Polarization

(a) A HCl molecule possesses a permanent dipole moment $p_0$.
(b) In the absence of a field, thermal agitation of the molecules results in zero net average dipole moment per molecule.
(c) A dipole such as HCl placed in a field experiences a torque that tries to rotate it to align $p_0$ with the field $E$.
(d) In the presence of an applied field, the dipoles try to rotate to align with the field against thermal agitation. There is now a net average dipole moment per molecule along the field.

Complex Relative Permittivity
(related to time response)

\[ \varepsilon_r = \varepsilon'_r - j \varepsilon''_r \]

\[ \varepsilon_r = \text{dielectric constant} \]
\[ \varepsilon'_r = \text{real part of the complex dielectric constant} \]
\[ \varepsilon''_r = \text{imaginary part of the complex dielectric constant} \]
\[ j = \text{imaginary constant } \sqrt{-1} \]
Dielectric Loss Factor

Loss Tangent (related to energy loss)

$$\tan \delta = \frac{\varepsilon''}{\varepsilon'}$$

$\tan \delta$ = loss tangent or loss factor, $\varepsilon'_r$ = real part of the complex dielectric constant, $\varepsilon''_r$ = imaginary part of the complex dielectric constant

(a) An ac field is applied to a dipolar medium. The polarization $P(P = Np)$ is out of phase with the ac field.
(b) The relative permittivity is a complex number with real ($\varepsilon_r'$) and imaginary ($\varepsilon_r''$) parts that exhibit frequency dependence.
Example: Water Molecule

[Diagram of a water molecule with polarization indicated]

www.lsbu.ac.uk/water/molecule.html
Microwave Dielectric Relaxation of Liquid Water

- Dielectric relaxation indicated by:
  - Decrease in real permittivity
  - Peak in imaginary permittivity
- Maximum $\varepsilon''$ corresponds to maximum conversion from EM energy to thermal energy.
- High $\varepsilon''$
  - Good for microwave oven
  - Bad for device

Why not 20 GHz operation for a microwave oven?

- Open bands
  - 915 MHz (not all countries)
  - 2.45 GHz
  - 5.8 GHz
  - 24.1 GHz
- Cost constraints
Water in a proton exchange membrane

- Current PEM fuel cells are based on PSA membranes, e.g. Nafion. The essential feature of Nafion is the nano-separation of hydrophilic/hydrophobic domains


Why not characterize water in porous glass in this way?
(a) A crystal with equal number of mobile positive ions and fixed negative ions. In the absence of a field, there is no net separation between all the positive charges and all the negative charges.
(b) In the presence of an applied field, the mobile positive ions migrate toward the negative charges and positive charges in the dielectric. The dielectric therefore exhibits interfacial polarization.
(c) Grain boundaries and interfaces between different materials frequently give rise to interfacial polarization.

Space Charge in Ceramic Capacitors with Glass

- Need long enough time for charge to move to boundary

\[ \tau \propto \frac{d}{\sigma} \]

\( d = \text{grain size} \)

Grain boundary or interface

Relaxation Time

Grain Size

Grain Conductivity
Glass is of major importance as an bond between ceramic and metal, and a filler.

Glass is of major importance as an additive to ceramics in order to promote sintering at low temperature.
BaTiO$_3$ Ceramics with Glass boundaries

Relaxation time = 0.0001 s

Figure shows dielectric response of a BaTiO3 – Glass composite

From the relaxation time and microstructure, we can determine the grain conductivity

Janosik Thesis
Frequency Response of Dielectric Polarization

\[ \varepsilon'_r \leq 10000 \]

- Interfacial and space charge

\[ \varepsilon'_r \leq 100 \]
- Orientational, Dipolar

\[ \varepsilon'_r \leq 30 \]

\[ n = \varepsilon'_r \leq 4 \]

- Ionic
- Electronic

Focus on Microwave region

\[ \varepsilon'_r = 1 \]

\[ 10^2 \quad 1 \quad 10^2 \quad 10^4 \quad 10^6 \quad 10^8 \quad 10^{10} \quad 10^{12} \quad 10^{14} \quad 10^{16} \]

- Radio
- Infrared
- Ultraviolet light

Fig 7.15

Table 7.2 Typical examples of polarization mechanisms

<table>
<thead>
<tr>
<th>Example</th>
<th>Polarization</th>
<th>Static $\varepsilon_r$</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar gas</td>
<td>Electronic</td>
<td>1.0005</td>
<td>Small $N$ in gases: $\varepsilon_r \approx 1$</td>
</tr>
<tr>
<td>Ar liquid ($T &lt; 87.3$ K)</td>
<td>Electronic</td>
<td>1.53</td>
<td>van der Waals bonding</td>
</tr>
<tr>
<td>Si crystal</td>
<td>Electronic polarization due to valence electrons</td>
<td>11.9</td>
<td>Covalent solid; bond polarization</td>
</tr>
<tr>
<td>NaCl crystal</td>
<td>Ionic</td>
<td>5.90</td>
<td>Ionic crystalline solid</td>
</tr>
<tr>
<td>CsCl crystal</td>
<td>Ionic</td>
<td>7.20</td>
<td>Ionic crystalline solid</td>
</tr>
<tr>
<td>Water</td>
<td>Orientational</td>
<td>80</td>
<td>Dipolar liquid</td>
</tr>
<tr>
<td>Nitromethane (27 °C)</td>
<td>Orientational</td>
<td>34</td>
<td>Dipolar liquid</td>
</tr>
<tr>
<td>PVC (polyvinyl chloride)</td>
<td>Orientational</td>
<td>7</td>
<td>Dipole orientations partly hindered in the solid</td>
</tr>
</tbody>
</table>

$\text{BaTiO}_3$ permittivity (dielectric constant) = 1,000
Permittivity of Amorphous Materials

Permittivity values are related to the electron density and an ionic charge

- SiO$_2$ $\varepsilon_r=4$
- Commercial flat panel Ba-Si-O $\varepsilon_r=8$
- 40%Ba-20%Ti-40%Si-0 $\varepsilon_r=15$
- Ta$_2$O$_5$ $\varepsilon_r=25$
- Nb$_2$O$_5$ $\varepsilon_r=40$
- Mainly electronic and ionic contributions
Frequency (or time) Response

• Relaxation Response
  – Based on diffusion mechanisms
  – Significant damping in oscillations
  – Describes Dipolar and Space charge mechanisms

• Resonance Response
  – High frequency response
  – Not as much damping as relaxation response
(a) Real and imaginary part is of the dielectric constant, $\varepsilon_r'$ and $\varepsilon_r''$ versus frequency for (a) a polymer, PET, at 115 °C and (b) an ionic crystal, KCl, at room temperature.
both exhibit relaxation peaks but for different reasons.

SOURCE:

Summary of Dielectric Response

• 4 basic mechanisms with each mechanism having a characteristic frequency response

• Glasses potentially have electronic, ionic and space charge contributions

• Highest permittivity for a glass is less than 20

• Discussion point – is rotational polarization possible in glass?
Metamaterials

Mike Lanagan, Khalid Rajab, Masato Iwasaki, Doug Werner and Elena Semouchkina

Materials Research Institute
Penn State University
Metamaterials Reading assignment
Metamaterials  
(Based on negative permittivity)

• Description and Definition of Metamaterials

• Discovery and Application

• Creating materials with a resonant response
  – Plasmonic resonances for optics (not covered here)
  – Dielectric Resonators (interesting for Microwave and THz)

• Why Glass is an Interesting Medium for Metamaterials
  – Low dielectric loss
  – Easy to create spheres and periodic structures
  – Particular interest for mm-wave and THz frequencies
Electromagnetic Cloaking Using Metamaterials

*J.B. Pendry et al., Science 312, 1780 (2006).*
LEFT-HANDED $\varepsilon<0$ AND $\mu<0$ METAMATERIALS

Veselago, 1960s

$\varepsilon > 0, \mu > 0$  
Regular Materials  
(right-handed)

$\varepsilon < 0, \mu < 0$  
Backward Waves  
Left-handed Materials

$n = -\sqrt{\varepsilon \mu}$

Negative-Refractive-Index (NRI) Materials

George V. Eleftheriades//University of Toronto
NEGATIVE REFRACTION

Negative-Refractive-Index (NRI) Media

\[
\frac{\sin \theta_1}{\sin \theta_2} = n
\]

George V. Eleftheriades//University of Toronto
Negative Index of Refraction

Image appears on opposite side

Meta-Material

Positive Index of Refraction

Image appears slightly closer

Natural Material
Discovery of Metamaterials

- Predicted by Veselago in 1960s
- First Experiments at UC San Diego in 2000
- Significant interest for applications
  - Magnetic resonant imaging
  - THz imaging
  - Cloaking
How can one make metamaterials?

• Think of resonance
  – Result of standing waves
  – Function of the wavelength and structure size

• We will use ring resonators as an example

Microwave: Resonator Size should be in **centimeters**

Resonant frequency \( f_r \) is given by:

\[
 f_r \propto \frac{1}{d\varepsilon_r}
\]

\( d=\text{Resonator size} \)
Apple iPhone and Microwaves

- **Quad-band GSM**
  - 850 MHz
  - 900 MHz
  - 1800 MHz
  - 1900 MHz

- **Bluetooth**
  - 2400 MHz

- **802.11 WiFi**
  - 2400 MHz
Ring Resonator Measurements

HP8510T Network Analyzer
45 MHz to 26 GHz

Intercontinental Microwave Fixture

Ring Resonator
1 cm
Resonant Behavior in Ring Resonators

Transmission Coefficient (dB)

<table>
<thead>
<tr>
<th>S21</th>
<th>(dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FDTD - experiment

K = 9.3

3D Frequency Domain Field Magnitude Second Resonant Peak 7.3 GHz

Electric Field perpendicular to substrate plane

3D Frequency Domain Field Magnitude First Resonant Peak 3.8 GHz

Simulations by L. Haney
Double Negative Materials*

Negative permeability results from the resonating magnetic element

Negative permeability results from the resonating electric element

Recall \( n = - (\varepsilon \mu)^{1/2} \)

Critical Experiment for Metamaterial

First make a metamaterial prism

Side View

Top View
Critical Experiment for Metamaterial

- Incident microwave direction
- Normal to plane of refraction
- Refracted beam direction for positive index
- Refracted beam direction for negative index
Experimental Confirmation of a Meta-material*

Metamaterial $n=-2.7$

Teflon $n=1.4$

R. A. Shelby et al., Science, pg. 77 (2001)
Why not other resonant structures for Metamaterials?

Ceramic Cylinders

Microwave ceramic resonators made by Murata

Glass Spheres

1 mm diameter silica spheres. Fabricated by Amanda Baker

Dielectric properties and geometry are key factors for resonators
Microwave Filter for Cell Phone Base Station: Commercial Application of Ceramic Dielectric Resonators

One frequency out

Many frequencies in
Microwave Characterization

Resonant Post

Brass Plate

Coupler

Dielectric Sample

Power In

Power Out
Resonant Post Method

Resonant Post Method

Power in

Brass Plate

Power Out

Coupler

Dielectric Sample

TE_{011} Mode

Frequency (GHz)

Power Out

HEM111

TE011

HEM211

TM011

HEM121

HEM311

*Hakke and Coleman, IEEE (1960)
# Field Distribution of TE$_{011}$ Mode from FDTD Simulation

<table>
<thead>
<tr>
<th>TE011</th>
<th>E-field</th>
<th>H-field</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Top-view</strong></td>
<td><img src="image1.png" alt="E-field Top-view" /></td>
<td><img src="image2.png" alt="H-field Top-view" /></td>
</tr>
<tr>
<td><strong>Side-view</strong></td>
<td><img src="image3.png" alt="E-field Side-view" /></td>
<td><img src="image4.png" alt="H-field Side-view" /></td>
</tr>
</tbody>
</table>

- **Dielectric resonator**
- **Metal plate**

M. Iwasaki
Masato “Mat” Iwasaki, Visiting Scientist
NGK Spark Plug

- Meta-materials
- Electromagnetic Simulation
Simulation and Experimental Results

(a) TE_{011} mode

(b) HEM_{111} mode

Source probe

Receiving probe

View from Top

Receiving angle /°

Normalized S_{21}

Simulation and Experimental Results

View from Top

Transmitted Power

Receiving Angle

50 A/m

Incident point

Receiving point

-90°

90°

HEM_{111}

TE_{011}
Electric field distribution of single DR

- By simulation results, magnetic field distributions were drawn in longitudinal direction at the half height of DR.

(a) TE_{011} mode

(b) HEM_{111} mode

(c) HEM_{211} mode

(d) HEM_{311} mode

M. Iwasaki
Field Distribution of Square DR Cluster

- Magnetic field distributions in longitudinal direction at the half height of DR were drawn.

**HEM\(_{111}\) mode**

No HEM \(_{111}\)
mode propagation
for square symmetry

**HEM\(_{211}\) mode**

HEM \(_{211}\)
mode propagation
for square symmetry
is consistent with
lattice symmetry

M. Iwasaki
Magnetic Field Symmetry in Dielectric Resonator Modes

TE\textsubscript{011} Mode

Field Distribution of Each Resonant Mode

<table>
<thead>
<tr>
<th>Mode</th>
<th>TE\textsubscript{011}</th>
<th>HEM\textsubscript{111}</th>
<th>HEM\textsubscript{211}</th>
<th>HEM\textsubscript{311}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Field</td>
<td>None</td>
<td>2-fold</td>
<td>4-fold</td>
<td>6-fold</td>
</tr>
</tbody>
</table>

Moving from individual resonators to clusters to arrays

- For characterizing the refracted waves through wedge-shaped DR arrays, Simulations and measurements starting from one DR will be performed.
- **Excitation with large area** should be employed.

Dielectric Resonator

Increasing the number of DRs to form wedge shape

: Incident waves

M. Iwasaki
Ceramic Dielectric Resonator Arrays

Top View
Resonator array
in a low permittivity matrix

Simulation by Elena Semouchkina

Operating
Frequency 15 GHz
Moving Beyond Microwaves

- **Materials Trends**
  - Higher application frequencies (both communications and computing)
  - Lower permittivity (dielectric constant) and lower loss (higher Q)
  - All dielectric (no metal?) structures

- **Design and Process Implications**
  - More compact designs
  - Dimensional control becomes more critical

- **Measurement Implications**
  - Optical methods
  - GPS
  - Bluetooth
  - Computers
  - Broadband and Data
  - Imaging & Astronomy

- **Lumped Elements**
  - Cellular Phone
  - Automotive Guidance

- **Distributed Elements**
  - 1GHz
  - 2GHz
  - 3GHz
  - 5GHz
  - 100GHz
  - 1THz

*http://www.fz-juelich.de/isg/isg2/isg2-sh/ebg_materials.htm*
**Systems Level:** Innovative devices for precision measurement, shielding, imaging, telecommunications, energy, and biomedicine

- **Novel Antennas**
- **MRI Systems**
- **THz Imaging**
- **Metamaterials for IR Devices**
- **Superlens-based Nanopatterning**
- **EM Cloaking**

*Fang et al., Science, 2005*
*Pendry et al., Science, 2006*
THz Characterization of Arrays

- **Materials:**
  - Silicon Nitride, Si$_3$N$_4$ \( \varepsilon_r \approx 8.9 \)
  - Brass

- **Lattices:**
  - Square
  - Hexagonal

- **Unit cells:**
  - 4mm
  - 3mm
  - 2mm

Blue – Measured resonant frequencies
Red – Scattering cross-section (Mie)

Khalid Rajab
What’s Next for Ceramic Dielectric Materials and Structures?

- Higher Frequencies pushing into the THz range
- What size resonators do we need?
- What types of dielectrics (glass?) do we need?

1 mm diameter silica spheres. Fabricated by Amanda Baker
Quiz

• What material property affects the resonator frequency?
• What other parameter affects resonance?
• Why would we NOT want to make the resonator too small?
• What functionalities of glass are potentially important for metamaterials?
Metamaterials in Magnetic Resonance Imaging?

- Overview of how MRI works
- Use of resonators in MRI (not metamaterials yet)
- Case Study: Glass Metamaterials for MRI
Background on Magnetic Resonance Imaging (MRI)

Magnetic resonance imaging is based on the absorption and emission of energy in the radio frequency range of the electromagnetic spectrum. Radio Frequency (RF) Coils are used to transmit and receive energy from the samples.

(Adapted from Reference: http://www.cis.rit.edu/htbooks/mri)
Background on MRI contd.

- MRI is based on spatial variations in the phase and frequency of the radio frequency energy being absorbed and emitted by the imaged object.
- Important microscopic property responsible for MRI is the spin property within hydrogen nuclei.
- The human body is primarily fat and water. Fat and water have many hydrogen atoms which make the human body approximately 63% hydrogen atoms.

(Adapted from Reference: http://www.cis.rit.edu/htbooks/mri)
7 Tesla MRI device at the NMR spectroscopy lab

Andrew Webb Penn State University
Schematic MRI System

Strong dc magnetic field (B0)

= Time varying transverse field (B1) produced by the RF coils
Depending on the magnetic field the rf field varies between 100 and 1,000
Imaging a Canola Seed

Ceramic Cylinder as an MRI insert

Canola Seed Image

Elena Semouchkina, Varun Tyagi, Michael Lanagan, Amanda Baker, Andrew Webb, Thomas Neuberger
Case Study

• Design a resonator for a 3Tesla MRI
• Frequency = 300 MHz
Case Study

- First think of the wavelength for the resonator replacing RF coil insert
- What will be size of the glass resonator
  - How do we shrink the size
  - Do you think that loss is important?

Block diagram of MRI Equipment
The frequency dependence of the real and imaginary parts of the dielectric constant in the presence of interfacial, orientational, ionic, and electronic polarization mechanisms.

\[ \varepsilon' \leq 100 \]
\[ \varepsilon' \leq 30 \]
\[ n = \varepsilon' \leq 4 \]

**Focus on Microwave region**

**Radio**  \[ 10^2 \]
**Infrared**  \[ 10^8 \]
**Ultraviolet light**  \[ 10^{16} \]
How do we make a high permittivity glass?

$$\varepsilon_r = 1 + \frac{N\alpha_e}{\varepsilon_o}$$

$\varepsilon_r$ = relative permittivity

$N$ = number of molecules per unit volume

$\alpha_e$ = electronic polarizability

$\varepsilon_o$ = permittivity of free space

Assumption: Only ionic and electronic polarization is present

Summary of glass as a dielectric

• Dielectric response for glass occurs over a wide frequency range
• New applications for dielectrics could involve glass
• Functionality of glass
  – Related to dielectric properties (permittivity and loss
  – Formability and cost
Dielectric Loss and Q Factor

Loss Tangent \[ \tan \delta = \frac{\varepsilon''_r}{\varepsilon'_r} \]

Q Factor \[ Q = \frac{1}{\tan \delta} = \frac{\text{energy \_ stored}}{\text{energy \_ dissipated}} \]

\( \varepsilon'_r = \) real part of the complex dielectric constant, \( \varepsilon''_r = \) imaginary part of the complex dielectric constant