PERMITTVITY AND PERMEABILITY AND THE BASIS OF EFFECTIVE PARAMETERS[*]

James Baker-Jarvis, Michael D. Janezic, Bill Riddle, Ronald C. Wittmann
National Institute of Standards and Technology
325 Broadway, Boulder, CO

Abstract

The concepts of effective permittivity and permeability are used throughout the literature to describe heterogeneous materials, inhomogeneous materials, and small collections of molecules. In this paper we study definitions of the permittivity and permeability based on the microscopic Maxwell's equations and then discuss the ramifications of the common usage of the term "effective".

Introduction

The goal of this paper is to critically evaluate the concept of effective permittivity and permeability at both the macroscopic and microscopic scales. We will concentrate on the permittivity, but the permeability would follow a similar path.

The permittivity is the constitutive parameter that relates the macroscopic time-harmonic electric field to the macroscopic displacement field $\mathbf{D} = \varepsilon\ \mathbf{E}$. If we consider electromagnetic wave propagation from macroscopic, to mesoscopic, to molecular scales, the effective response at each level is related to different degrees of homogenization. The concept of permittivity critically depends on how the inhomogeneities are treated. There have been many types of ensemble and volumetric averaging methods used to derive the macroscopic fields from the microscopic fields (see Jackson and the reference therein [1]). For example, in the most commonly used theory, materials are averaged at a molecular level to produce effective molecular dipole moments. Then these effective moments are assumed to form a continuum, which then forms the basis of the macroscopic polarization. The procedure assumes that the wavelength in the material is much larger than the particle sizes. As Jackson [1] notes: the macroscopic Maxwell's equations can model refraction and reflection of visible light, but not X-ray diffraction and therefore he states that the length scale $L_0 = 1 \times 10^{-8}$ m is the lower limit for the validity of the macroscopic equations. The microscopic electromagnetic theories developed in Jackson [1] replace the averaged molecular multipoles,

with averaged point multipoles usually located at the center-of-mass position. This approach works well down to near the molecular level, but breaks down at the molecular to submolecular level. Also, for macroscopic heterogeneous materials the effective dipole moments of the inclusions must be treated as the effective molecular moments, and the wavelengths of the fields must adhere to these criteria. When this criterion does not hold then the spatial derivatives in Maxwell's equations are not well defined and the displacement field loses its meaning. Associated with this homogenization process at a given frequency is the number of molecules or inclusions that are required to define a displacement field and thereby the related permittivity. Definitions of the permittivity of plasmas and artificial structures will be analyzed.

Macroscopic, Mesoscopic, and Microscopic Descriptions

The microscopic Maxwell equations are $\partial\mathbf{B}/\partial t = -\nabla \Box\ \mathbf{E}$, $\varepsilon_0\ \mu_0\ \partial\mathbf{E}/\partial t = \nabla \Box\ \mathbf{B} - \mu_0\ \mathbf{j}_m$, $\nabla\bullet\ \mathbf{B} = 0$, and $\nabla\bullet\ \mathbf{E} = \rho_m$, where ρ_m and j_m are the microscopic charge density and current density due to elementary charges and its motion. In order to form the displacement field $\mathbf{D}$ that appears in the macroscopic Maxwell's equations, we need to expand the ensemble-averaged charge density in a Taylor series as $<\rho_m\ (r, t)> \approx\ \rho(r,t) - \nabla \bullet \mathbf{P}\ (r,t) + ...$ where the first term in the series is identified as the macroscopic charge density ρ and the second term on the RHS defines the macroscopic polarization $\mathbf{P} = <\sum \mathbf{p}_n\ \delta(x - x_n\ )>$, where $\mathbf{p}_n$ are the effective molecular moments. Higher order terms in the Taylor series can be neglected only when $k\ L_0 \Box 1$, where $k = 2\pi/\lambda$. Using this procedure the displacement can be defined as $\mathbf{D} = \varepsilon_0\mathbf{E} + \mathbf{P}$ [1]. The macroscopic magnetic field $\mathbf{H}$ is formed through a Taylor series expansion of the microscopic current density that contains the macroscopic current density and magnetic polarization $\mathbf{M}$, which yields $\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$. Through these averaging procedures we obtain the macroscopic Maxwell equations $\partial\mathbf{B}/\partial t = -\nabla \Box\ \mathbf{E}$, $\partial\mathbf{D}/\partial t = \nabla \Box\ \mathbf{H} - j$, $\nabla\bullet\ \mathbf{B} = 0$, $\nabla\bullet\ \mathbf{D} = \rho$. The main feature we need to point out is that the Taylor series approximation depends on a long wavelength assumption where $kL_0 \Box 1$. The displacement vector needs to originate from a statistical model from the microscopic Maxwell equations. In addition, the permittivity must be an analytic, causal function that satisfies $\varepsilon(-\omega) = \varepsilon^*(\omega)$. In the constitutive modeling process, the key constituents are the polarization and macroscopic fields. From a

macroscopic aspect, the impulse- response function is used to express the most general linear relation between the displacement and electric fields

$$\mathbf{D}(t) = \varepsilon_0 \mathbf{E}\,(t) + \int f_p(\tau)\,\mathbf{E}(t\text{-}\tau)\,d\tau\,,$$

where $f_p(t)$ is the polarization impulse-response function and the permittivity is defined as $\varepsilon(\omega) = \varepsilon_0 + \int f_p(\tau)\,e^{-i\omega\tau}d\tau$. From this perspective the constitutive relationships delegate the effects of the microstructure into the definition of the impulse-response function in the time domain or the permittivity and permeability in the frequency domain. From a statistical mechanical approach the polarization is defined as

$$\mathbf{P}(t) = \iint <d\mathbf{P}(t)/dt\ \ \mathbf{P}(\tau)> \bullet \mathbf{E}\,(\tau)\,d\tau\,dV/k_BT,$$

where $<>$ denotes averaging over a distribution function. We see that on a microscopic level the polarization has its basis in correlations between microscopic dipole moments. This requires a sample size large enough, relative to wavelength, that a probability density can be defined to homogenize the fields. From a statistical-mechanical aspect the permittivity evolves from Laplace transforms of the pulse-response or the correlation functions whose real part are related to fluctuations and the imaginary part is related to losses due to intermolecular collisions.

There are two approaches that are commonly used for dielectric measurements on discontinuous or heterogeneous media. The first is a rigorous method of matching the tangential components of the fields at all discontinuous interfaces. This approach cannot be used for complicated materials structures. The second method involves a homogenization process that assumes that the media is continuous and the applied field has a long wavelength relative to inclusion size.

Near the resonant frequency the breakdown in effective media theories will vary depending on the effects of multiple scattering. There are two classes of resonances in dielectrics. The first is a mechanical resonance where the resonant frequency between molecules or atoms is modeled by Hooke's law with a resonance frequency $\omega = (k_h/m)^{1/2}$, where k_h is the force constant. These resonant frequencies generally occur at wavelengths much, much larger than the particle size and therefore do no invalidate the permittivity concept. The second type of resonance is a geometric resonance that occurs when the inclusion size is comparable to one-half wavelength or where there are resonances in passive devices embedded in

the material. When wavelengths approach inclusion size then geometric resonances occur and the statistical averaging procedure is less apparent. Many authors use the term effective permittivity even when the wavelength in the material approaches the inclusion sizes and geometrical resonances occur.

Numerical Modeling

We consider a specimen of length L that partially fills the length of a coaxial line. We examine the effective relative permittivity that is obtained as we include larger and larger amounts of the air regions in the coaxial line as part of the effective length of the sample. The top curve is polyfluorotetraethylene (PTFE) measured alone. We see, as expected, that as the sample length increases due to increasing air region included with the sample, the "effective" permittivity decreases. Non-physical behavior is manifested in the oscillations due to one-half wavelength geometric resonances
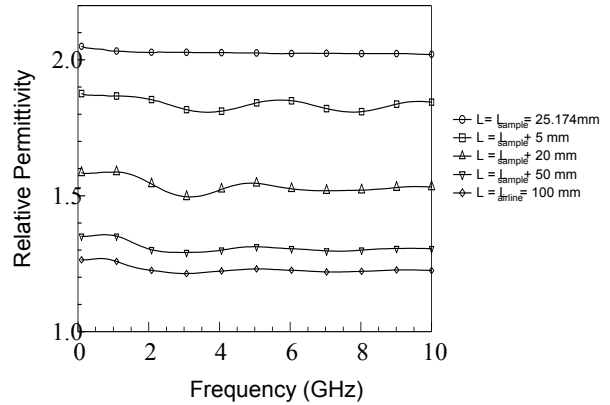

Fig. 1: Measurements of PTFE in a coaxial waveguide for various effective lengths.

Discussion

The definitions of the permittivity and the displacement function require that $kL_0 \square\ 1$ and the behavior must also be causal. Our simple example of an effective media in a coaxial line highlights nonphysical behavior that may result near geometrical resonances with different permittivities.

References

[1]   J. D. Jackson, *Classical Electrodynamics*, Wiley, NY, 1999