

---

This is an electronic reprint of the original article.  
This reprint may differ from the original in pagination and typographic detail.

Author(s): Sihvola, Ari

Title: Dielectric Polarization and Particle Shape Effects

Year: 2007

Version: Final published version

**Please cite the original version:**

Sihvola, Ari. 2007. Dielectric Polarization and Particle Shape Effects. Journal of Nanomaterials. Volume 2007. P. 1-9. ISSN 1687-4110 (printed). DOI: 10.1155/2007/45090.

Note: Copyright © 2007 Ari Sihvola. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

---

All material supplied via Aaltodoc is protected by copyright and other intellectual property rights, and duplication or sale of all or part of any of the repository collections is not permitted, except that material may be duplicated by you for your research use or educational purposes in electronic or print form. You must obtain permission for any other use. Electronic or print copies may not be offered, whether for sale or otherwise to anyone who is not an authorised user.

## Review Article

# Dielectric Polarization and Particle Shape Effects

**Ari Sihvola**

*Electromagnetics Laboratory, Helsinki University of Technology, P.O. Box 3000, 02015 TKK, Finland*

Received 15 February 2007; Revised 30 April 2007; Accepted 30 May 2007

Recommended by Christian Brosseau

This article reviews polarizability properties of particles and clusters. Especially the effect of surface geometry is given attention. The important parameter of normalized dipolarizability is studied as function of the permittivity and the shape of the surface of the particle. For nonsymmetric particles, the quantity under interest is the average of the three polarizability dyadic eigenvalues. The normalized polarizability, although different for different shapes, has certain universal characteristics independent of the inclusion form. The canonical shapes (sphere, spheroids, ellipsoids, regular polyhedra, circular cylinder, semisphere, double sphere) are studied as well as the correlation of surface parameters with salient polarizability properties. These geometrical and surface parameters are essential in the material modeling problems in the nanoscale.

Copyright © 2007 Ari Sihvola. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

## 1. INTRODUCTION

The engineering strive towards always smaller scales in the structure of matter is obvious even to people who are not working in the field of materials science. The sole terminology and use of words in popularization of technological progress may lead us to think that microelectronics is somewhat old-fashioned; nanotechnology is the theme of tomorrow if not yet today. Progress is indeed great. If measured in the exact meaning of prefixes, it is thousandfold.

This trend of looking in smaller details happens on several fronts. Scientists want to understand the structure of matter in nanoscales, engineers wish to control structures with always sharper technological tools, research program plans dream of the multiplied possibilities of material responses that this tailoring can provide, and the public expects new and unseen applications of technology along with the increased degrees of freedom.

What does the penetration of technology into smaller scales mean in terms of materials modeling? In particular, how does it affect the analysis of the electromagnetic properties of composites? The modeling of the effective properties of heterogeneous materials requires knowledge about the properties of the constituent materials and about the geometrical arrangements how these phases together compose the continuum. Classical homogenization approaches are based on a quasistatic principle. In other words, the electromagnetic field solutions are calculated using Laplace's and

Poisson's equations instead of the full Maxwell's equations. This means that the response of an individual scatterer is instantaneous. No retardation effects are needed over the size of the scatterer.

If the modeling is hence based on the assumption that the reaction of a single inclusion is like in statics and its size is considerably smaller than the wavelength of the operating electromagnetic field, the road towards smaller scales of the individual scatterers would not cause any additional problems. On the contrary, for a given electromagnetic excitation, the locally quasistatic assumption becomes more and more acceptable.

How, then, does the nanoscale modeling of heterogeneous materials differ from that of microscale or mesoscale? Certainly, many of the applied principles remain the same. And the science of materials modeling has provided us very detailed theories to predict the macroscopic dielectric characteristics of media (for a comprehensive historical review of these theories, see [1]). This is because the governing laws of electromagnetics are valid over a broad range of spatial and temporal scales. Of course, there is a limit since matter is not infinitely divisible. In the "very small nanoscale," the inclusions are clusters in which the macroscopic response is partially determined by discreteness of the building block atoms. For example, quantum confinement may affect band gap sizes in semiconductors and lasers. But in this article we are not yet manipulating individual atoms and do not take into account the granularity of matter. Let us concentrate on

such nanoscale environments where a typical object would be measured in tens of nanometers. This is much larger than the atomic dimensions which are of the order of angstroms ( $10^{-10}$  meters). The classic expression from 1959 by Richard P. Feynman, “*there’s plenty of room at the bottom,*” is astonishingly still valid in the era of nanotechnology [2].

But there is another view at the effect of scaling. Not all remain the same when the amplification in our microscope is increased and we are dealing with objects of smaller dimension. A sphere remains a sphere, be it small or large, but some of its characteristic parameters change relative to each other, even if we now neglect the discreteness that ultimately has to be faced when moving to molecular scales. Also in the continuum treatment, the specific surface area of the sphere (or of any other reasonable object for that matter) increases in direct proportion to the scale decrease: the area of the sphere surface divided by the sphere volume is inversely proportional to the radius. Then it is to be expected that the surface effects start to dominate when we are moving from the ordinary-sized material textures into the smaller-scale structures. The increased focus on surfaces of individual scatterers also means that in the modeling of composites and other heterogeneous materials composed of these type of inclusions, the interaction effects between neighboring scatterers need more attention than in connection to larger-scale modeling. Interaction forces are not scale-independent. At the same time as the surface area relative to the volume for a given particle increases, its surface-area-to-weight ratio increases with a similar pace.

In this article, the basic materials modeling questions are discussed in connection to the dielectric properties of matter. Because of the generality of the electric modeling results, many of the results are, *mutatis mutandis*, directly applicable to certain other fields of science, like magnetic, thermal, and even (at least analogously) mechanical responses of matter. In the chapters to follow, special emphasis is given to the manner how geometric and surface characteristics affect the response of clusters. Many of the results to be presented have been published in my previous special articles that concern the dielectric response of particles of various shapes. This review connects those results and discusses the surface-geometrical parameters of various particle polarizabilities that are of importance in the modeling of material effects in the nanoscale.

## 2. ELECTRIC RESPONSE OF A SPHERICAL SCATTERER

Many materials modeling approaches and theories are based on the principle of splitting the analysis into two parts: the whole is seen as composed of a collection of single scatterers whose response is first to be calculated (or if the mixture is composed of many different phases, the responses of all of these phases are needed), and then the global, macroscopic properties have to be computed as certain interactive sums of all the component inclusions.

Let us next focus on the first step in this process: the response of an individual, well-defined inclusion. The quasi-static response parameters of a given object can be gleaned

from the solution of the problem when the object is placed in vacuum and exposed to a uniform static electric field.

The simplest shape is a sphere. And the simplest internal structure is homogeneity. The response of a homogeneous, isotropic, dielectric sphere in a homogeneous, uniform electric field in vacuum is extraordinary simple: it is a dipolar field. And the internal field of the sphere is also uniform, directed along the exciting field and of an amplitude dependent on the permittivity. No higher-order multipoles are excited.

The relations are: the homogeneous internal field  $\vec{E}_i$  as a function of the exciting, primary field  $\vec{E}_e$  reads [3, 4]

$$\vec{E}_i = \frac{3\epsilon_0}{\epsilon + 2\epsilon_0} \vec{E}_e, \quad (1)$$

where  $\epsilon$  is the (absolute) permittivity of the spherical object and  $\epsilon_0$  the free-space permittivity. Then obviously the polarization density induced within the sphere volume is  $(\epsilon - \epsilon_0)\vec{E}_i$  and since the dipole moment of a scatterer is the volume integral of the polarization density (dipole moment density), the dipole moment of this sphere is

$$\vec{p} = (\epsilon - \epsilon_0) \frac{3\epsilon_0}{\epsilon + 2\epsilon_0} \vec{E}_e V, \quad (2)$$

where  $V$  is the volume of the sphere. And from this relation follows the polarizability of the sphere  $\alpha$ , which is defined as the relation between the dipole moment and the incident field ( $\vec{p} = \alpha\vec{E}_e$ ):

$$\alpha = 3\epsilon_0 V \frac{\epsilon - \epsilon_0}{\epsilon + 2\epsilon_0}. \quad (3)$$

This polarizability is an extremely important characteristic quantity in modeling of dielectric materials. It is true that polarizability does not tell the whole story about the response of a scatterer. In case of inclusion, shapes other than spherical,<sup>1</sup> also quadrupolic, octopolic, and even higher-order multipoles are created (and in the case of dynamic fields, the list of multiple moments is much longer, see [5] for a concise treatment of these). Perhaps a more accurate name for the polarizability we are now discussing would be dipolarizability.

Why is this (di)polarizability so essential? In other words, what makes the dipole moment so distinct from the other multipole moments? Part of the answer is that the effect of the multipoles on the surroundings decreases with the distance in an inverse power. And the higher is the power, the higher is the order of the multipole. Therefore, the greatest far-field effect is that of the lowest multipole. Dipole is the lowest-order multipole except monopole. And monopole is not counted since a monopole requires net charge, and we are here dealing with neutral pieces of matter which have equal amounts of positive and negative charges.

<sup>1</sup> And in the spherical case, too, when the exciting electric field is nonuniform, the perturbational field is not purely dipolar.

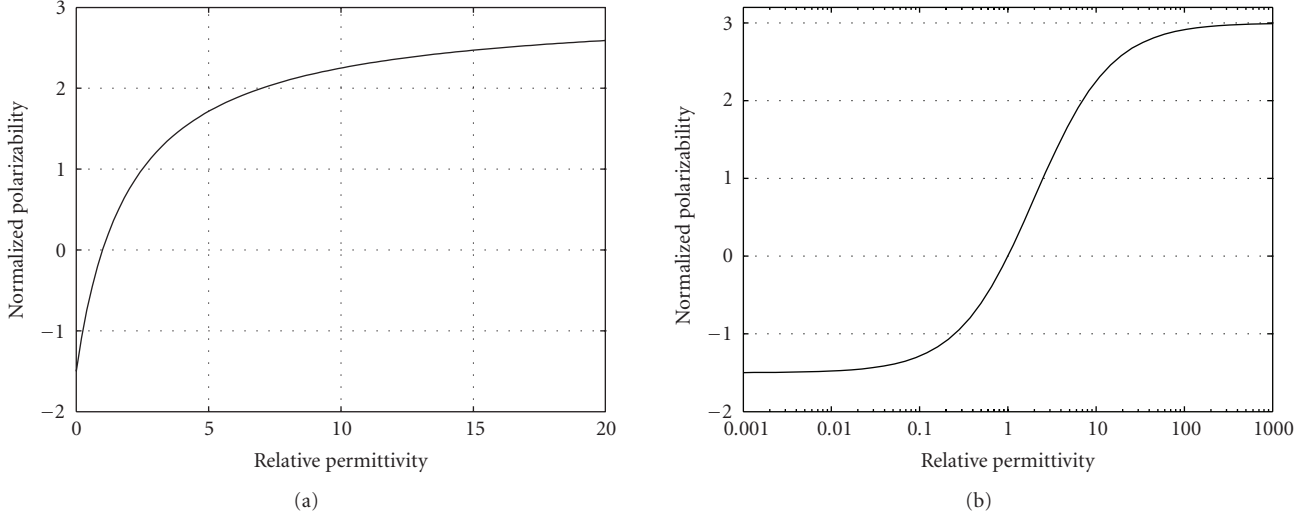


FIGURE 1: The polarizability of a dielectric sphere for positive values of the relative permittivity, with linear and logarithmic scales. Note the negative values for the polarizability for permittivities less than that of free space. The symmetry of the polarizability behavior in the two limits (high-permittivity, or “conducting” and zero-permittivity, or “insulating”) can be seen from the right-hand side curve.

Therefore, let us concentrate on the (di)polarizability  $\alpha$ . As can be seen from (3), there is a trivial dependence of the polarizability on the volume. Obviously, the bigger the volume of the inclusions is, the larger its electrical response is. A more characteristic quantity would be a normalized polarizability  $\alpha_n$ , which for the sphere reads

$$\alpha_n = \frac{\alpha}{\epsilon_0 V} = 3 \frac{\epsilon_r - 1}{\epsilon_r + 2}, \quad (4)$$

where the dimensionless quality of this quantity is guaranteed by the division with the free-space permittivity  $\epsilon_0$ . Note also the use of the relative permittivity of the sphere  $\epsilon_r = \epsilon/\epsilon_0$ .

Here is the response of matter stripped to the very essentials. It is a response quantity of the most basic three-dimensional geometrical object with one single material parameter, permittivity. And still, this response function is by no means trivial. Some of the properties of this function are very universal as we will see later.

Figure 1 displays the polarizability behavior of a dielectric sphere for positive permittivity values. The obvious limits are seen: the saturation of the normalized polarizability to the value 3 for large permittivities and to the value  $-3/2$  for the zero-permittivity.

But it is not unfair to note that the polarizability function in Figure 1 seems rather monotonous and dull. However, if the permittivity is freed from the conventional limits within the domain of positive values, very interesting phenomena can be observed. To display this, Figure 2 is produced.

In Figure 2, one phenomenon overrides all other polarizability characteristics: the singularity of the function for the permittivity value  $\epsilon_r = -2$ , directly appreciated from (4). This is the electrostatic resonance that goes in the literature under several names, depending on the background of the authors, which can be electromagnetics, microwave engi-

neering, optics, or materials science. This is the surface plasmon or Fröhlich resonance [6].

However, the present article does not concentrate on negative-permittivity materials. Metamaterials [7] form a large class of media that embrace such negative-permittivity media and metamaterials in fact are very much in the focus of today’s research [8, 9]. In the following, let us restrict ourselves to positive permittivity values. Interesting results can be extracted about the material response also within this regime.

Let us collect some of these basic observations that are most clearly seen from the formula for the polarizability of the sphere (4), but also valid for other dielectric objects in the three-dimensionally averaged sense [10]. The normalized polarizability  $\alpha(\epsilon_r)$ , for the permittivity value  $\epsilon_r = 1$ , satisfies the following:

- (i)  $\alpha = 0$  at  $\epsilon_r = 1$ ,
- (ii)  $\partial\alpha/\partial\epsilon_r = 1$  at  $\epsilon_r = 1$ ,
- (iii)  $\partial^2\alpha/\partial\epsilon_r^2 = -2/3$  at  $\epsilon_r = 1$ .

Indeed, the polarizability is a quite powerful tool in analyzing the dielectric response of single scatterers but also the response of dielectric mixtures as a whole. The classical homogenization principles starting from Garnett [11], following through Bruggeman [12], over to the modern refined theories take careful respect to the polarizabilities of the inclusions that make up the mixture they are modeling.

Let us next allow the geometry of the inclusion deviate from the basic spherical shape.

### 3. ELLIPSOIDS AND NONSYMMETRY

To gather more information about how the microgeometry and the specific surface area have effect on the material response of dielectric scatterers, let us allow the spherical

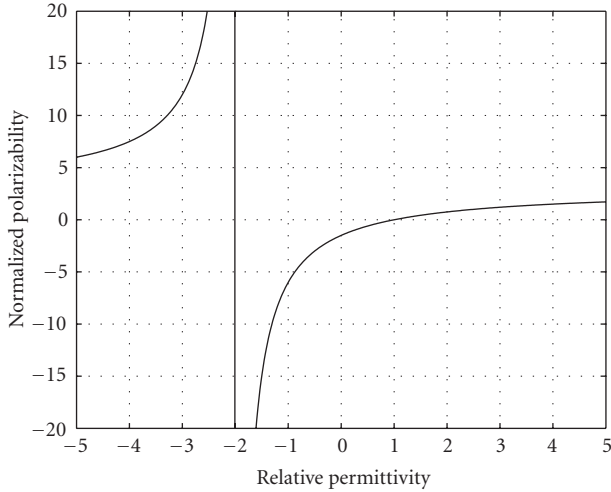


FIGURE 2: The polarizability of a dielectric sphere when the permittivity is allowed to be negative as well as positive.

form to be changed to ellipsoid. Ellipsoids are easy geometries since the dipole moment of such shaped homogeneous objects can be written in a closed form, which is a consequence of the fact that the internal field of a homogeneous ellipsoid in a constant electric field is also constant.<sup>2</sup> The amplitude of this field is naturally linear to the external field, but there also exists a straightforward dependence of this field on the permittivity of the ellipsoid and of a particular shape parameter, so-called depolarization factor.

Let the semiaxes of the ellipsoid in the three orthogonal directions be  $a_x, a_y, a_z$ . Then the internal field of the ellipsoid (with permittivity  $\epsilon$ ), given that the external, primary field  $\vec{E}_e$  be  $x$ -directed, is (a generalization of (1))

$$\vec{E}_i = \frac{\epsilon_0}{\epsilon_0 + N_x(\epsilon - \epsilon_0)} \vec{E}_e, \quad (5)$$

where  $N_x$  is the depolarization factor of the ellipsoid in the  $x$  direction, and can be calculated from

$$N_x = \frac{a_x a_y a_z}{2} \int_0^\infty \frac{ds}{(s + a_x^2) \sqrt{(s + a_x^2)(s + a_y^2)(s + a_z^2)}}. \quad (6)$$

For the other depolarization factor  $N_y$  ( $N_z$ ), interchange  $a_y$  and  $a_x$  ( $a_z$  and  $a_x$ ) in the above integral.<sup>3</sup>

The three depolarization factors for any ellipsoid satisfy

$$N_x + N_y + N_z = 1. \quad (7)$$

<sup>2</sup> Note, however, that the field *external* to the ellipsoid is no longer purely dipolar. In the vicinity of the boundary, there are multipolar disturbances whose amplitudes depend on the eccentricity of the ellipsoid.

<sup>3</sup> A Java applet to calculate the depolarization factors and polarizability components of an arbitrary ellipsoid is located in the URL address of the Helsinki University of Technology <http://users.tkk.fi/~mpitkone/Ellipsoid/Ellipsoidi.html>

A sphere has three equal depolarization factors of  $1/3$ . For prolate and oblate spheroids (ellipsoids of revolution), closed-form expressions can be written for the depolarization factors [4, 13]. The limiting cases of spheroids are disk (depolarization factors  $(0, 0, 1)$ ) and a needle (depolarization factors  $(1/2, 1/2, 0)$ ).

From the field relation (5), the normalized polarizability components follow. In this case where the spherical symmetry is broken, the polarizabilities are different for different directions. In the  $x$ -direction, the polarizability component reads

$$\alpha_{n,x} = \frac{\epsilon_r - 1}{1 + N_x(\epsilon_r - 1)} \quad (8)$$

and the corresponding expressions for the  $y$ - and  $z$ -components are obvious. This relation allows quite strong deviations from the polarizability of the spherical shape. For a simple example, consider the limits of very large or very small permittivities. These read

- (i)  $\alpha_{n,x} = 1/N_x$ , for  $\epsilon_r \rightarrow \infty$ ,
- (ii)  $\alpha_{n,x} = -1/(1 - N_x)$ , for  $\epsilon_r \rightarrow 0$ .

And obviously these may possess wild limits when the depolarization factors have the allowed ranges  $0 \leq N_i \leq 1$  for any of the three components  $i = x, y, z$ . This hints to the possibilities that with extremely squeezed ellipsoids one might be able to create strong macroscopic effective responses, at least if the field direction is aligned with all the ellipsoids in the mixture.

In addition to the view at the special polarization properties of a mixture composed of aligned ellipsoids, the isotropic case is also very important. An isotropic mixture can be generated from nonsymmetric elements (like ellipsoids) by mixing them in random orientations in a neutral background. Then the average response of one ellipsoid is a third of the sum of its three polarizability components:

$$\alpha_{n,ave} = \frac{1}{3} \sum_{i=x,y,z} \frac{\epsilon_r - 1}{1 + N_i(\epsilon_r - 1)}. \quad (9)$$

The effect of the eccentricity (nonsphericity) of the ellipsoid is visible from Figure 3 where the average polarizability is plotted against the permittivity for different ellipsoids.

#### 4. ARBITRARY SHAPE OF THE INCLUSION

If the inclusion has a shape other than the ellipsoid, the electrostatic solution of the particle in the external field does not have a closed-form solution. Fortunately, for such cases, very efficient computational approaches have been developed. With various finite-element and difference-method principles, many electrostatics and even electromagnetic problems can be solved with almost any desired accuracy (see, e.g., [14, 15]).

Then also the polarizabilities of these arbitrarily shaped particles can be found. For an arbitrary object, there are now new geometrical parameters that define the inclusion and which affect the polarizability, in addition with the permittivity. One of the interesting questions in connection with

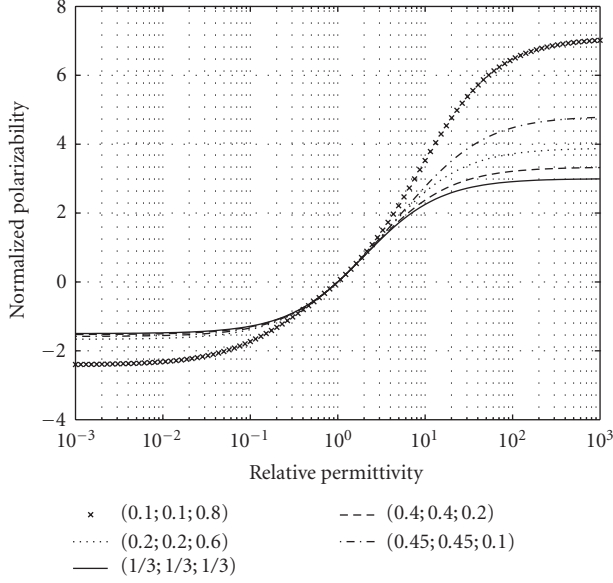


FIGURE 3: The average polarizability of a dielectric ellipsoid (one-third of the normalized polarizabilities in the three orthogonal directions) for various depolarization factor triplets.

nanostructures is how the specific geometrical and surface parameters correlate with the amplitude of the polarizability. A systematic study into this problem would require the numerical electrostatic analysis of very many different scatterer shapes. And again for those shapes that are nonsymmetric<sup>4</sup>, one needs to distill the trace (or the average of the components) of the polarizability dyadic, which in the end would be a fair quantity to compare with the canonical shapes.

Let us review some of the important shapes for which there does not exist a closed-form solution of the Laplace equation, or such one only exists in a form of infinite series. The parameter that tells the essentials about the response is the normalized polarizability. In the normalized form, the linear dependence on the volume of the inclusion is taken away, and the effect of geometry is mixed with the effect of permittivity.

#### 4.1. Platonic polyhedra

Perhaps the most symmetric three-dimensional shapes after sphere are the five regular polyhedra: tetrahedron, hexahedron (cube), octahedron, dodecahedron, and icosahedron. They share with the sphere the following property: the polarizability dyadic is a multiple of the unit dyadic. In other words, the three eigenvalues of polarizability are equal. One single parameter is sufficient to describe the dipole moment

response. Of course, higher-order multipolarizabilities are also present in increasing magnitudes as the sharpness of the corners of the polyhedra increases.

The dielectric response of these regular Platonic objects have been solved with a boundary-integral-equation principle [16]. An integral equation for the potential is solved with method of moments [17] which consequently allows many characteristic properties of the scatterer to be computed. Among them, the polarizabilities of the five Platonic polyhedra have been enumerated with a very good accuracy. Also regression formulas turned out to predict the polarizabilities correct to at least four digits. These have been given in the form [16]

$$\alpha_n = \alpha_\infty (\epsilon_r - 1) \frac{\epsilon_r^3 + p_2 \epsilon_r^2 + p_1 \epsilon_r - \alpha_0}{\epsilon_r^4 + q_3 \epsilon_r^3 + q_2 \epsilon_r^2 + q_1 \epsilon_r + \alpha_\infty}, \quad (10)$$

where  $p_1, p_2, q_1, q_2, q_3$  are numerical parameters, and  $\alpha_\infty$  and  $\alpha_0$  are the computationally determined polarizability values for  $\epsilon_r \rightarrow \infty$  and  $\epsilon_r \rightarrow 0$ , respectively. Of course, these parameters are different for all five polyhedra. At the special point  $\epsilon_r = 1$ , the conditions  $\alpha_n = 0, \alpha'_n = 1, \alpha''_n = -2/3$  are satisfied for all five cases. See also [10] for the connection of the derivatives of the polarizability with the virial coefficients of the effective conductivity of dispersions and the classic study by Brown [18] on the effect of particle geometry on the coefficients.

Figure 4 shows the polarizabilities of the various shapes as functions of the permittivity.<sup>5</sup> From these results it can be observed that the dielectric response is stronger than that of the sphere, and the response seems to be stronger for shapes with fewer faces (tetrahedron, cube) and sharper corners, which is intuitively to be expected. Sharp corners bring about field concentrations which consequently lead to larger polarization densities and to a larger dipole moment.

#### 4.2. Circular cylinder

Another basic geometry is the circular cylinder. This shape is more difficult to analyze exhaustively for the reason that it is not isotropic. The response is dependent on the direction of the electric field. The two eigendirections are the axial direction and the transversal direction (which is degenerate as in the transverse plane, no special axis breaks the symmetry). Furthermore, the description of the full geometry of the object requires one geometrical parameter (the length-to-diameter ratio) which means that the two polarizability functions are dependent on this value and the dipolarizability response of this object is a set of two families of curves depending on the permittivity.

With a computational approach, the polarizabilities of circular cylinders of varying lengths and permittivities have

<sup>4</sup> Nonsymmetric in the sense that the polarizability operator has three distinct eigenvectors; perhaps it is not proper to call such scatterers anisotropic because anisotropy is commonly associated with the direction dependence of the bulk material response.

<sup>5</sup> A Java-applet to calculate the depolarization factors and polarizability components of Platonic polyhedra is located in the URL address of the Helsinki University of Technology  
<http://www.tkk.fi/Yksikot/Sahkomagnetikka/kurssit/animaatio/Polarisaatio.html>

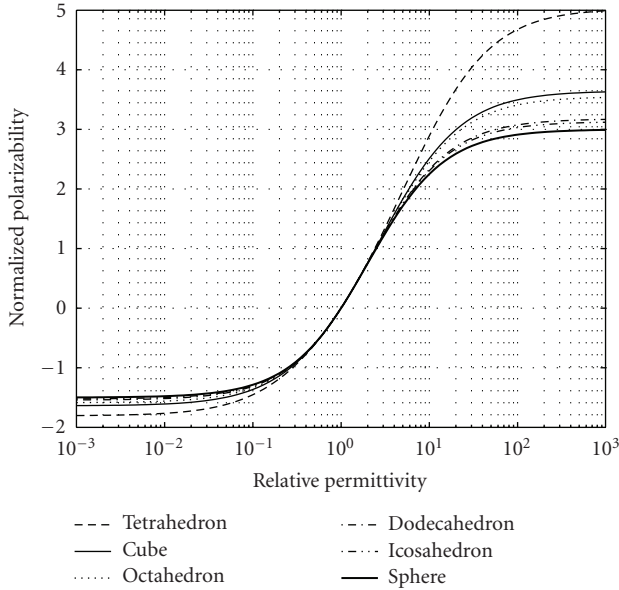


FIGURE 4: The polarizabilities of Platonic polyhedra and sphere. Note that the curve for sphere is always smallest in magnitude, and the order of increase is icosahedron, dodecahedron, octahedron, hexahedron, and tetrahedron (which has the highest curve).

been computed [19]. Again, approximative formulas give a practical algorithm to calculate the values of the polarizabilities. In [19], these formulas are given as differences to the polarizabilities of spheroids with the same length-to-width ratio as that of the cylinder under study. Spheroids are easy to calculate with exact formulas (8). Since they come close to cylinders in shape when the ratio is very large or very small, probably their electric response is also similar, and the differences vanish in the limits. Obviously, the field singularities of the wedges in the top and bottom faces of the cylinder cause the main deviation of the response from that of the spheroid. Note also [20] and the early work on the cylinder problem in the U.S. National Bureau of Standards (see references in [15]).

An illustrative example is the case of “unit cylinder.” A unit cylinder has the height equal to the diameter [21]. Its polarizability components are shown in Figure 5. There, one can observe that its effect is stronger than that of sphere (with equal volume), but not as high as that of a cube.

### 4.3. Semisphere

A dielectrically homogeneous semisphere (a sphere cut in half gives two semispheres) is also a canonical shape. However, the electrostatic problem where two dielectrically homogeneous domains are separated by semispherical boundaries lead to infinite series with Legendre functions. The polarizability of the semisphere cannot be written in a closed form. However, by truncating the series and inverting the associated matrix, accurate estimates for the polarizability can be enumerated [22]. This requires matrix sizes of a couple of hundred rows and columns. Furthermore, a semisphere as

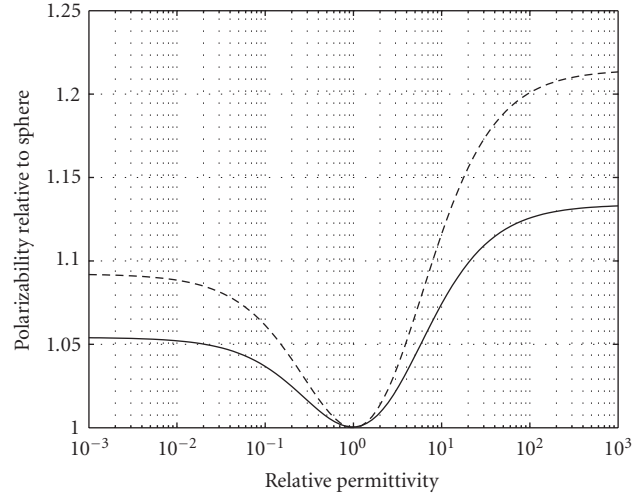


FIGURE 5: A comparison of the polarizability of a unit cylinder and cube. The unit cylinder has different response to axial and transversal excitations; here one-third of the trace of the polarizability is taken. Both curves are relative to a sphere with the corresponding volume and permittivity.

a rotationally symmetric object has to be described by two independent polarizability components. However, it is more “fundamental” than cylinder because no additional geometrical parameter is needed to describe its shape.

The axial ( $z$ ) and transversal ( $t$ ) polarizability curves for the semisphere resemble those for the other shapes. The limiting values for low and high permittivities are the following:

$$\begin{aligned} \alpha_{n,z} &\approx 2.1894, & \alpha_{n,t} &\approx 4.4303, & (\epsilon_r \rightarrow \infty) \\ \alpha_{n,z} &\approx -2.2152, & \alpha_{n,t} &\approx -1.3685, & (\epsilon_r \rightarrow 0). \end{aligned} \quad (11)$$

Note here the larger high-permittivity polarizability in the transversal direction compared to the longitudinal, which is explained by the elongated character in the transversal plane of the semisphere. However, in the  $\epsilon_r = 0$  limit, the situation is the opposite: a larger polarizability for the axial case (larger in absolute value, as the polarizability is negative).

### 4.4. Double sphere

A very important object especially in the modeling of random nanomaterials is a doublet of spheres. A sphere is a common, equilibrium shape. And when a sphere in a mixture gets into the vicinity of another sphere, especially in the small scales the interaction forces may be very strong, and the doublet of spheres can be seen as a single polarizing object. Even more, two spheres can become so closely in contact that they merge and metamorphose into a cluster. Such a doublet can be described with one geometrical parameter: the distance between the center points of the spheres divided by their radius. The value 2 for this parameter divides the range into

the two cases whether the doublet is clustered or separate. Again, this object is rotationally symmetric and needs to be described by two polarizabilities, axial and transversal.

A solution of the electrostatic problem with double-sphere boundary conditions is not easy. It requires either a numerical approach or a very complicated analysis using toroidal coordinate system. Several partial results have been presented for the problem [23–25], but only recently a full solution for this problem [26] and its generalization [27] have appeared.

In both limiting cases of the double sphere (the distance of the center points of the spheres goes either to zero or very large), both of the normalized polarizability components of the double sphere approach the sphere value (4). And obviously, it deviates from the sphere value to a largest degree when the distance between the centers is around two radii (the distance for maximum deviation depends on the permittivity of the spheres). For the case of  $\epsilon_r$  approaching infinity, the case of touching spheres has the following analytical properties [25, 28]:

$$\alpha_{n,z} = 6\zeta(3) \approx 7.212; \quad \alpha_{n,t} = \frac{9}{4}\zeta(3) \approx 2.705 \quad (12)$$

with the Riemann Zeta function. Here the axial polarizability ( $z$ ) is for the case that the electric field excitation is parallel to the line connecting the center points of the two spheres, and if the field is perpendicular to it, the transversal ( $t$ ) polarizability applies.

## 5. CORRELATION OF THE POLARIZABILITY WITH SURFACE PARAMETERS

From the polarizability results in the previous section for various shapes of inclusions, it is obvious that in the polarizability characteristics, sphere is a minimum geometry. In other words, with a given amount of dielectric material, in a spherical form it creates the smallest dipole moment, and every deviation from this shape increases its polarizability.<sup>6</sup> Also theoretical results to prove this have appeared in the literature [28, 29]. But how does the deviation of the dielectric response from that of sphere depend on the geometrical difference between the object and sphere? This is a difficult question to answer because there are infinite number of ways how the shape of a spherical object can begin to differ from that perfect form.

But intuitively it seems reasonable that all information about the geometrical and surface details of various properties of object is encoded the polarizability curves. However, on the other hand, from a look at the curves for various objects, one might expect that the curves contain also very much redundant information. After all, they resemble

TABLE 1: Characteristic figures for the polarizability of Platonic polyhedra and sphere. Note the third derivative of  $\alpha_n$  at  $\epsilon_r = 1$ ; the first and second derivatives are equal for all objects.

	$\alpha_n(\epsilon_r = \infty)$	$\alpha_n(\epsilon_r = 0)$	$\alpha'_n(\epsilon_r = 0)$	$\alpha'''_n(\epsilon_r = 1)$
Tetrahedron	5.0285	-1.8063	4.1693	0.98406
Cube	3.6442	-1.6383	3.0299	0.82527
Octahedron	3.5507	-1.5871	2.7035	0.78410
Dodecahedron	3.1779	-1.5422	2.4704	0.71984
Icosahedron	3.1304	-1.5236	2.3659	0.70087
Sphere	3	-1.5	2.25	0.66667

each other very much in their global form. As was pointed out earlier, the polarizabilities of all isotropic scatterers seem to have equal values, and also equal-valued first and second derivatives at  $\epsilon_r = 1$ . Table 1 shows the values of the limiting polarizabilities and the derivative at  $\epsilon_r = 0$  and the third derivative at  $\epsilon_r = 1$  for the five polyhedra and sphere.

The results in Table 1 show also that the numerical correlations between the values of the third derivate and the limiting values at low and high permittivities are very high (of the order of 0.98 and more). Therefore, one could expect that it is possible to compress very much of the polarizability characteristics into a few characteristic numbers.

Article [30] contains a systematic study of comparing the amplitudes of the polarizabilities to certain well-defined geometrical properties of the deformed objects. For regular polyhedra, the following characteristics tell something about the object: number of faces, edges, vertices, solid angle subtended by the corners, specific surface area, and radii of the circumscribed and inscribed spheres. These have been correlated against the electrical polarizability parameters with interesting observations, among which the following is not unexpected: the polarizability of a perfect electric conductor ( $\epsilon_r \rightarrow \infty$ ) polyhedron correlates strongly with the inverse of the solid angle of the vertex. On the other hand, the strongest correlation of the polarizability of “perfectly insulating sphere” (in other words the case  $\epsilon_r = 0$ ) is with the normalized inscribed radius of the polyhedron.

## 6. DISCUSSION

A detailed knowledge of the polarizability of inclusions with basic shapes gives valuable information about the way such building blocks contribute to the effective dielectric parameters of a continuum. Many models for the macroscopic properties of matter replace the effect of the particles in the medium fully by its polarizability. It is to be admitted that for complex scatterers, this is only a part of the whole response which also contains near-field terms due to higher-order multipoles that is characterized by stronger spatial field variation close to the scatterer. Nevertheless, dipolarizability remains the dominant term in the characteristics of the inclusion.

<sup>6</sup> Here polarizability has to be understood in the average three-dimensional sense. Of course, some of the polarizability components of an ellipsoid may be smaller than that of the sphere of the same permittivity and volume; however, the remaining components are so much larger that the average will override the sphere value.



The shortcoming of the direct scaling of the macroscopic polarization results down to nanoscale is that the results discussed in this paper are based on quasistatic analysis and are therefore scale-independent. The modeling principles make use of the normalized polarizabilities of particles (like (4)). This remains constant even if we decrease the size of the particle. On the other hand, the specific surface area of an inclusion increases without limit when its size becomes small. Surface effects dominate in the nanoscale. Clusters more complex than the fairly basic shapes discussed in this paper are formed.

Of course, the translation of continuum models (like this analysis of basic shapes and their responses) into smaller scales is problematic also in another respect. Even if we are not yet in the molecular and atomic level in the length scales, this nanoregion is the intermediate area between bulk matter and discrete atoms. One cannot enter into very small scales without the need of quantum physical description. This deviation from the classical physics description is hiding behind the corner and we have to remember that exact geometrical shapes start to lose meaning in the deeper domains of nanoscale. Another issue to be connected to the manner how well the shapes remind of those familiar from continuum three-dimensional world, is whether the nanoclusters are built from exact ordered crystal structure or more amorphous-like aggregates. One could expect that in the latter case the “softer” forms (spheres and ellipsoids) would be more correct approximations to reality. And because the classical mixing rules very often rely on assumptions of such scatterer shapes, we might expect that homogenization and effective medium theories have their place also in materials modeling in the nanoscale.

## REFERENCES

- [1] C. Brosseau, “Modelling and simulation of dielectric heterostructures: a physical survey from an historical perspective,” *Journal of Physics D*, vol. 39, no. 7, pp. 1277–1294, 2006.
- [2] The transcript of Richard P. Feynman’s talk *There’s plenty of room at the bottom* at the annual meeting of the American Physical Society on December 29, 1959, is a classic reference in nanoscience, February 2007, <http://www.zyvex.com/nanotech/feynman.html>.
- [3] J. D. Jackson, *Classical Electrodynamics*, John Wiley & Sons, New York, NY, USA, 3rd edition, 1999.
- [4] A. Sihvola, *Electromagnetic Mixing Formulas and Applications*, IEE Publishing, London, UK, 1999.
- [5] R. E. Raab and O. L. de Lange, *Multipole Theory in Electromagnetism: Classical, Quantum, and Symmetry Aspects, with Applications*, Clarendon Press, Oxford, UK, 2005.
- [6] C. F. Bohren and D. R. Huffman, *Absorption and Scattering of Light by Small Particles*, John Wiley & Sons, New York, NY, USA, 1983.
- [7] A. Sihvola, “Electromagnetic emergence in metamaterials,” in *Advances in Electromagnetics of Complex Media and Metamaterials*, S. Zouhdi, A. Sihvola, and M. Arsalane, Eds., vol. 89 of *NATO Science Series: II: Mathematics, Physics, and Chemistry*, pp. 1–17, Kluwer Academic Publishers, Dordrecht, The Netherlands, 2003.
- [8] December 2006, <http://www.metamorphose-eu.org>.
- [9] DARPA stands for the *Defense Advanced Research Projects Agency* and is the central research and development organization for the U.S. Department of Defense (DoD), December 2006, <http://www.darpa.mil/dso/thrust/matdev/metamat.htm>.
- [10] E. J. Garboczi and J. F. Douglas, “Intrinsic conductivity of objects having arbitrary shape and conductivity,” *Physical Review E*, vol. 53, no. 6, pp. 6169–6180, 1996.
- [11] J. C. M. Garnett, “Colours in metal glasses and in metallic films,” *Philosophical Transactions of the Royal Society of London*, vol. 203, pp. 385–420, 1904.
- [12] D. A. G. Bruggeman, “Berechnung verschiedener physikalischer Konstanten von heterogenen Substanzen. I. Dielektrizitätskonstanten und Leitfähigkeiten der Mischkörper aus isotropen Substanzen,” *Annalen der Physik*, vol. 416, no. 7, pp. 636–664, 1935.
- [13] L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media*, Pergamon Press, Oxford, UK, 2nd edition, 1984.
- [14] A. Mejdoubi and C. Brosseau, “Finite-element simulation of the depolarization factor of arbitrarily shaped inclusions,” *Physical Review E*, vol. 74, no. 3, Article ID 031405, 13 pages, 2006.
- [15] M. L. Mansfield, J. F. Douglas, and E. J. Garboczi, “Intrinsic viscosity and the electrical polarizability of arbitrarily shaped objects,” *Physical Review E*, vol. 64, no. 6, Article ID 061401, 16 pages, 2001.
- [16] A. Sihvola, P. Ylä-Oijala, S. Järvenpää, and J. Avelin, “Polarizabilities of platonic solids,” *IEEE Transactions on Antennas and Propagation*, vol. 52, no. 9, pp. 2226–2233, 2004.
- [17] S. Järvenpää, M. Taskinen, and P. Ylä-Oijala, “Singularity extraction technique for integral equation methods with higher order basis functions on plane triangles and tetrahedra,” *International Journal for Numerical Methods in Engineering*, vol. 58, no. 8, pp. 1149–1165, 2003.
- [18] W. F. Brown, “Solid mixture permittivities,” *The Journal of Chemical Physics*, vol. 23, no. 8, pp. 1514–1517, 1955.
- [19] J. Venermo and A. Sihvola, “Dielectric polarizability of circular cylinder,” *Journal of Electrostatics*, vol. 63, no. 2, pp. 101–117, 2005.
- [20] M. Fixman, “Variational method for classical polarizabilities,” *The Journal of Chemical Physics*, vol. 75, no. 8, pp. 4040–4047, 1981.
- [21] A. Sihvola, J. Venermo, and P. Ylä-Oijala, “Dielectric response of matter with cubic, circular-cylindrical, and spherical microstructure,” *Microwave and Optical Technology Letters*, vol. 41, no. 4, pp. 245–248, 2004.
- [22] H. Kettunen, H. Wallén, and A. Sihvola, “Polarizability of a dielectric hemisphere,” Tech. Rep. 482, Electromagnetics Laboratory, Helsinki University of Technology, Espoo, Finland, February 2007.
- [23] B. U. Felderhof and D. Palaniappan, “Longitudinal and transverse polarizability of the conducting double sphere,” *Journal of Applied Physics*, vol. 88, no. 9, pp. 4947–4952, 2000.
- [24] L. Poladian, “Long-wavelength absorption in composites,” *Physical Review B*, vol. 44, no. 5, pp. 2092–2107, 1991.
- [25] H. Wallén and A. Sihvola, “Polarizability of conducting sphere-doublets using series of images,” *Journal of Applied Physics*, vol. 96, no. 4, pp. 2330–2335, 2004.
- [26] M. Pitkonen, “Polarizability of the dielectric double-sphere,” *Journal of Mathematical Physics*, vol. 47, no. 10, Article ID 102901, 10 pages, 2006.

- 
- [27] M. Pitkonen, "An explicit solution for the electric potential of the asymmetric dielectric double sphere," *Journal of Physics D*, vol. 40, no. 5, pp. 1483–1488, 2007.
- [28] M. Schiffer and G. Szegő, "Virtual mass and polarization," *Transactions of the American Mathematical Society*, vol. 67, no. 1, pp. 130–205, 1949.
- [29] D. S. Jones, "Low frequency electromagnetic radiation," *IMA Journal of Applied Mathematics*, vol. 23, no. 4, pp. 421–447, 1979.
- [30] A. Sihvola, P. Ylä-Oijala, S. Järvenpää, and J. Avelin, "Correlation between the geometrical characteristics and dielectric polarizability of polyhedra," *Applied Computational Electromagnetics Society Journal*, vol. 19, no. 1B, pp. 156–166, 2004.