Correlation between the geometrical characteristics and dielectric polarizability of polyhedra

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Abstract

This article analyzes polarizability characteristics of the five regular polyhedra (tetrahedron, cube, octahedron, dodecahedron, and icosahedron) and sphere. In particular, the variation of the polarizabilities (polarizability is the amplitude of the static dipole moment caused by an incident electric field of unit amplitude) is correlated with various geometrical parameters of these Platonic solids: specific surface, number of edges, vertices, and faces, and the volumes of inscribed and circumscribed spheres. It is found that the polarizabilities of perfect electric conductor (PEC) and perfect electric insulator (PEI) objects are most strongly correlated with two different parameters: the radius ratio of circum- and inscribed spheres (PEC case) and the normalized radius of the inscribed sphere (PEI case).

1 Introduction

When a dielectric inclusion is put into a homogeneous and static electric field, there will be a perturbation in the behavior of the field function in the vicinity of the inclusion. The strongest component of this "scattered" field is that due to a (static) electric dipole moment $\mathbf{p}$. This dipole field is proportional to the incident uniform field $\mathbf{E}$. The proportionality coefficient is called polarizability α:

$$\mathbf{p} = \alpha \mathbf{E}_e. \tag{1}$$

For example, for a dielectric sphere with volume V and permittivity ϵ, the polarizability is [1, 2]

$$\alpha_s = 3V\epsilon_0 \frac{\epsilon - \epsilon_0}{\epsilon + 2\epsilon_0} \tag{2}$$

where ϵ_0 is the free-space permittivity (the permittivity of the environment in which the inclusion is embedded). Let us define the normalized dimensionless polarizability by

$$\alpha_n = \frac{\alpha}{\epsilon_0 V} \tag{3}$$

whence it is $\alpha_{n,s} = 3(\epsilon_r - 1)/(\epsilon_r + 2)$ for a sphere with relative permittivity ϵ_r. The two extreme cases are a PEC (perfect electric conductor, $\epsilon_r = \infty$) and PEI (perfect electric insulator, $\epsilon_r = 0$) inclusions:

$$\alpha_{n,s,\mathrm{PEC}} = 3, \quad \alpha_{n,s,\mathrm{PEI}} = -3/2. \tag{4}$$

In this paper, we will focus on the polarizabilities of inclusions with certain special basic shapes: in addition to the sphere also the five Platonic polyhedra (tetrahedron, hexahedron (cube), octahedron, dodecahedron, and icosahedron) are under consideration. As reported in [3], we have conducted an extensive study of the static polarizabilities of these shapes, and numerical values for these polarizabilities are now available to an accuracy of the order of 10^{-5}. Based on the calculations of [3], the estimates in Table 1 have been found for the normalized polarizabilities of Platonic polyhedra of the PEC and PEI type. The calculations were made by solving the surface integral equation for the potential function with Method of Moments and third-order basis functions.

The numerical values of Table 1 tell that the polarizability amplitude values for the PEC and PEI cases are correlated: a "sharper" object, like the tetrahedron, has stronger polarizabilities (in both cases) than smoother ones, and the smoothest shape is obviously the sphere.[1] However, the amplitudes of these polarizabilities vary slightly differently in the two cases as can be seen in Figure 1, where they are plotted on the same PEC/PEI graph.

The aim in the present paper is to try to find correlation of the polarizability values with various geometrical characteristics of the polyhedra. The normalized polarizabilities for the limiting cases of PEC and PEI are correlated against several parameters which intuitively could be anticipated to have effect on the creation of the dipole moment. The geometrical parameters that are treated are the number of faces, edges, and vertices of the polyhedron, the solid angle subtended by the faces when looked inside from a vertex, the specific surface of the inclusion, as also various parameters connected with the spheres inscribed and circumscribed on the polyhedron. All these parameters vary from one polyhedron to another, and they can be thought as certain measures

[1] In fact, sphere is an extremum shape which has the minimum polarizability, given the permittivity and volume of the inclusion. Any deviation from this form will increase, averaged over all directions, the dipole field [4].

of “non-sphericity” or “unsmoothness.” However, each of the parameters measure this abstract sharpness property in a different way. It is therefore very interesting to see which of the geometrical characteristic figures varies most similarly with the polarizabilities.

Although the connection between the polarizabilities of regular polyhedra and their basic geometrical characteristics is interesting from the general mathematical nature, the electric polarizabilities are very important also from the practical point of view in modeling of materials. In practically all models for the effective permittivity of inhomogeneous media, polarizability is the mostly determining parameter. For dilute mixtures, the effective permittivity is linearly dependent on it and for higher loadings of the inclusion phase, the effect of the polarizability becomes nonlinear and more pronounced.

The objects of the present study, polyhedra, are very natural forms. On microscopic scale, solid-state matter takes its shape in basic regular crystal forms which makes good reason and need for the results of polarizabilities of polyhedra. And even if on a larger scale matter may be disordered, polycrystal or even amorphous and isotropic, the microscopic objects retain the basic structure. Then also the polarizabilities of the basic forms are essential when modelling the macroscopic response of such matter.

Furthermore, the results for electric polarizabilities are readily available for magnetic modeling of materials. This is thanks to the duality between the electric and magnetic problems; hence the exact analogy between permittivity and permeability on one hand and the electric and magnetic polarizabilities on the other.

2 Calculation of the polarizabilities with the method of moments

Let us suppose that a dielectric inclusion is put into a uniform z-directed incident field $\mathbf{E}_e = E_e \mathbf{u}_z$. The corresponding electrostatic field problem can be formulated as an integral equation for the unknown surface potential function ϕ [5]:

$$\begin{aligned}\phi_e(\mathbf{r}) \quad = \quad & \frac{\tau+1}{2}\phi(\mathbf{r}) + \\ & \frac{\tau-1}{4\pi}\int_S \phi(\mathbf{r}')\frac{\partial}{\partial n'}\left(\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right) dS', \\ & \mathbf{r} \text{ on } S. \end{aligned} \tag{5}$$

Here S is the surface of the inclusion, $\phi_e = -E_e\, z$ is the incident potential, $\tau = \epsilon_i/\epsilon_e$ is the ratio of the permittivities of the inclusion and exterior, respectively, and $\mathbf{n}'$ is the outward normal vector to the surface at point $\mathbf{r}'$.

Once the potential is known on the surface, the dipole moment $\mathbf{p}$ can be calculated by

$$\mathbf{p} = -(\tau-1)\epsilon_e \int_S \phi(\mathbf{r})\mathbf{n}(\mathbf{r})\, dS \tag{6}$$

and the polarizability α is obtained from (1).

The potential function that is needed in the estimation of the polarizability can be calculated by solving integral equation (5) with the method of moments (MoM) [6]. Let us suppose that the surface S is divided into planar triangular elements. Then the unknown potential ϕ is expressed as a linear combination of continuous high order polynomial basis functions $u_n^{(q)}$ defined on these elements [3]

$$\phi = \sum_{n=1}^{N} c_n u_n^{(q)}. \tag{7}$$

Here $q = 1, 2, \ldots$, is the order of a basis function. Using Galerkin’s method equation (5) is next multiplied by testing functions $u_m^{(q)}$, $m = 1, \ldots, N$, and integrated over S. The resulting set of equations can be written as the following matrix equation

$$A\, c = b, \tag{8}$$

where $c = [c_1, \ldots, c_N]^T$ is the unknown coefficient vector of ϕ.

Equation (5) is a Fredholm integral equation of the second kind with a weakly singular kernel. However, for non-smooth surfaces, like a tetrahedron or a cube, the order of the singularity of the kernel increases at the edges and corners. To improve the efficiency of the numerical algorithm, the integrals with singularities are evaluated in closed form. This method is based on the singularity extraction technique, originally introduced by Wilton et. al. [7] and Graglia [8] for linear basis functions, and more recently, generalized for high order polynomial basis functions in [9]. After the singular term is integrated analytically, the outer integral with respect to $\mathbf{r}$ and the other terms are regular and can be evaluated by standard numerical methods, for example with Gaussian quadrature. The singularity extraction technique clearly improves the accuracy of the calculation of the near interaction terms of the system matrix, and thus, leads to a more stable algorithm than pure numerical integration. The method also improves the accuracy of the near-singular terms, not only the singular ones.

Other factors that effect to the accuracy of the solution are e.g. mesh density and type of the basis functions. Since the potential ϕ varies strongly near the corners of S [10], an appropriate refinement of the mesh, which takes into account the behavior of the potential at the edges and corners, usually increases the accuracy. A couple of mesh refinements were tested in [3] and it was found that a mesh with a square root refinement towards the edges gives the best results. Also higher order basis function representations improve the numerical accuracy. Both second and third order basis functions were tested in [3], and the third order ones gave better results.

As is already pointed out, equation (5) is a Fredholm integral equation of the second kind. When iterative solvers are applied to solve such equations, usually accurate results are obtained within a few iterations. This seems to be the case when the matrix equation (8) is solved iteratively with the restarted version of the GMRES method [11] and τ is small. However, for high $\tau > 100$, the convergence dramatically slows down and in some cases the method does not converge at all. The reason is that equation (5) does not have a unique solution if the inclusion is PEC, i.e., if $\tau = \infty$. This non-uniqueness problem can be avoided, for example, by adding a constant value $1/N$ to each element of the matrix A [12]. Numerical experiments have demonstrated that by this simple modification the convergence can be essentially improved for inclusions with high τ values.

3 Polarizabilities and characteristic figures

Let us next list and define several geometrical parameters that could be interpreted as an abstract distance from sphericalness. For all five polyhedra and the sphere, these are correlated against each other in the figures to follow. Since there are five polyhedra, there are six points in the figures.

Table 2 gives various fundamental geometrical characteristics of the regular polyhedra. These are the number of faces, edges, and vertices. One further measure is the "sharpness" of the vertex, defined by the solid angle which is bounded by the faces when one looks into the polyhedron.[2] Note that on the table, sphere is also taken to be a special case of a Platonic polyhedron, having an infinite number of faces, edges, and vertices. Also, for the sphere, the solid angle seen from the vertex (that is, on any point on the surface of the sphere) is obviously half of the total solid angle, $4\pi/2 = 2\pi$.

Table 3 collects some other, more indirect, geometrical parameters of the polyhedra. The edge length a of each of the polyhedra is normalized such that the volume is unity. The parameters are

- the specific surface of the polyhedron, defined as the area of the surface of the object when its volume is unity (e.g., for a cube, edge length $a = 1$ gives unit volume, meaning that the surface is $6a^2 = 6$),
- the ratio of the radii of the circumcribed sphere $R_{\rm circ}$ and the inscribed sphere $r_{\rm in}$,
- the normalized equivalent radii of the circumscribed and inscribed spheres, $g_{\rm circ}$ and $g_{\rm in}$. These two equivalent radii are defined with the volumes of the circum- and inscribed spheres with

$$g_{\rm circ} = \left(\frac{V_{\rm circ}}{V}\right)^{1/3}, \quad g_{\rm in} = \left(\frac{V}{V_{\rm in}}\right)^{1/3} \tag{9}$$

  where V is the volume of the given polyhedron. Note that both are defined to be larger than unity.

It is tempting to predict that the polarizabilities of the various polyhedra follow the pattern of these characteristic parameters that measure how "nonspherical" or "sharp-formed" the polyhedra are. Let us try to make a graphical and quantitative estimation of this correlation.

In Figures 2–5, the geometrical parameters are plotted against the PEC and PEI polarizabilities of the objects.

A numerical measure for the correlation between two sets of parameter variables is the correlation coefficient ρ, defined by the following [13]:

$$\rho = \frac{\frac{1}{6}\sum_{i=1}^{6}(x_i - m_x)(y_i - m_y)}{\sqrt{\frac{1}{6}\sum_{i=1}^{6}(x_i - m_x)^2 \;\cdot\; \frac{1}{6}\sum_{i=1}^{6}(y_i - m_y)^2}} \tag{10}$$

where the six cases (five polyhedra and the sphere) are all included in the summation. The two variables, x and

[2] There are different ways to calculate the vertex solid angle. Perhaps the most elegant is the following (Girard's theorem): given the dihedral angles between the faces, the solid angle is the excess angle of the sum of the dihedral angles over the corresponding planar polygon angle-sum. This property is used in Table 2.

y (with arithmetic means m_x and m_y) represent any pair of the polarizabilities and the characteristic geometrical parameters listed above.

The correlation coefficients between the parameters are collected in Tables 4 and 5.

4 Conclusions

The trivial hypothesis that both polarizabilities (PEC and PEI) correlate with the geometrical "sharpness" parameters of the polyhedra is obviously confirmed by the constellation of points in Figures 2–5 and even more by the correlation numbers.[3] But certainly also more non-trivial conclusions can be drawn from the above results.

Firstly, it is conspicuous that the PEC and PEI polarizabilities behave differently (although the correlation coefficient between them is numerically quite high, 0.9901, as shown in Figure 1). The difference reflects the fact that there are various mechanisms that are causing the dipole moment creation, and therefore also the geometry and its parameters stand in different relation to the polarizabilities in the two cases.

It seems that the polarizability of the PEI sphere correlates more strongly with some of the geometrical parameters than the polarizability of the PEC sphere (in average, the correlation coefficients are higher for the PEI plots). We can observe that the strongest correlation exists between the normalized inradius $g_{\rm in}$ and the PEI polarizability of the objects ($\rho = 0.9977$), and also the PEI polarizability correlates quite well with the specific surface of the object ($\rho = 0.9957$). On the other hand, the best correlation of PEC polarizability is with the circumscribed–inscribed sphere radius ratio ($\rho = 0.9953$), the other good correlation being with the inverse of the solid angle seen from the vertex of the object ($\rho = 0.9937$).

It may be difficult to find hard physics from statistical numbers. However, some qualitative, yet significant, observations can be made. First, it is perhaps not totally foolish to connect the solid angle of the vertex of a polyhedron with the polarizability of a perfectly conducting object. In terms of a dielectric polarizability, the contrast between the object and the environment is extreme in such case. On a sharp vertex, charge is concentrated.[4] Hence the polarizability increases in the PEC case as the vertex solid angle decreases. On the other hand, in the PEI case the situation is the opposite: the external side of the polyhedron is "more conducting" and again the contrast is infinite. But the convex form of the polyhedra does not allow any sharp corners into the object. In the PEI case, then the properties of the inscribed sphere, rather than the sharpness of the vertices, are more essential parameters witht respect to the polarizability.

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References

[1] J.D. Jackson, *Classical Electrodynamics*, Third Edition, John Wiley, New York, 1999.

[2] A. Sihvola, *Electromagnetic Mixing Formulas and Applications*, IEE Publishing, Electromagnetic Wave Series 47, London, 1999.

[3] A. Sihvola, P. Ylä-Oijala, S. Järvenpää, J. Avelin: Polarizabilities of Platonic solids. To appear in *IEEE Transactions on Antennas and Propagation*, 2004.

[4] M. Schiffer and G. Szegö: Virtual mass and polarization, *Transactions of the American Mathematical Society*, Vol. 67, pp. 130-205, 1949.

[5] J. Van Bladel: *Electromagnetic Fields*, New York, Hemisphere Publishing Corporation, 1985. Revised edition.

[6] R. F. Harrington: *Field Computation by Moment Methods*, Macmillan, New York, 1968.

[7] D. R. Wilton, S. M. Rao, A. W. Glisson, D. H. Schaubert, O. M. Al-Bundak and C. M. Butler: Potential integrals for uniform and linear source distributions on polygonal and polyhedral domains. *IEEE Transactions on Antennas and Propagation*, Vol. 32, pp. 276-281, March 1984.

[8] R. D. Graglia, On the numerical integration of the linear shape functions times the 3-D Green's function or its gradient on a plane triangle: *IEEE Transactions on Antennas and Propagation*, Vol. 41, pp. 1448-1455, October 1993.

[3] To be sure, not all geometrical parameters fall in the same order as the polarizabilities. The increasing behavior of the six points is not strictly monotonous in some of the plots. The sharpness of the vertices is one example: icosahedron has sharper corners (smaller solid angle) than dodecahedron, even it is more "spherical" in most other respects; the same goes for octahedron and hexahedron (the solid angle of the vertex of the octahedron is smaller than in a cube).

[4] The field components and the charge density vary as $r^{\nu-1}$ with r being the distance from a conical conducting corner. For sharp corners, ν is close to zero [1, Section 3.4], and the dependence is quite singular.

[9] 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, pp. 1149-1165, 2003.

[10] J. Avelin, R. Sharma, I. Hänninen, and A. H. Sihvola: Polarizability analysis of cubical and square-shaped dielectric scatterers: *IEEE Transactions on Antennas and Propagation*, Vol. 49, No. 3, pp. 451-457, March 2001.

[11] Y. Saad and M. H. Schultz: GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems, *SIAM Journal of Scientific and Statistical Computing*, Vol. 7, pp. 856-869, 1986.

[12] M. S. Hämäläinen and J. Sarvas: Realistic conductivity geometry model of the human head for interpretation of neuromagnetic data, *IEEE Transactions on Biomedical Engineering*, Vol. 36, No. 2, February 1989.

[13] L. Råde and B. Westergren: *Mathematics Handbook for science and engineering*, Studentlitteratur, Lund, 1995.

Bio-sketches

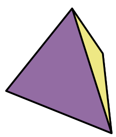
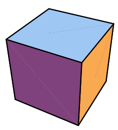
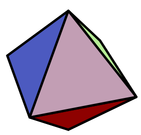
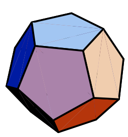
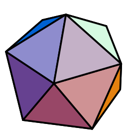
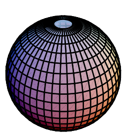
Ari Sihvola is professor of electromagnetics at Helsinki University of Technology (HUT), Espoo, Finland. He received the degree of Doctor of Technology from HUT in 1987, and has been a visiting scientist and professor at the Massachusetts Institute of Technology (1985–1986), the Pennsylvania State University (1990-1991), Lund University (1996), and the Swiss Federal Institute of Technology, Lausanne (2000–2001). Ari Sihvola is vice-chairman of the Finnish National Committee of URSI (the International Union of Radio Science).

Pasi Ylä-Oijala received the M.Sc. degree in 1992 and the Ph.D. degree in 1999, both in applied mathematics in the University of Helsinki, Finland. Since October 2002 he has been working as a researcher in Electromagnetics Laboratory, Helsinki University of Technology, Finland. His field of interest includes numerical techniques in computational electromagnetics based on the integral equation methods.

Seppo Järvenpää was born in 1965 received the M.Sc. degree in 1992 and the Ph.D degree in 2001, both in applied mathematics in the University of Helsinki, Finland. Currently he is working as a reseacher in the Electromagnetics Laboratory at Helsinki University of Technology. His field of interest include numerical techniques in computational electromagnetics based on finite element and integral equation methods.

Juha Avelin received the degree of Diploma Engineer in 1999, in Electrical Engineering, from Helsinki University of Technology. He is now working as researcher in the Electromagnetics laboratory of HUT. His current research interests are homogenization of mixtures and canonical problems in electromagnetics.

Table 1: Limiting values ($\epsilon_r \to \infty$, PEC; and $\epsilon_r \to 0$, PEI) for the normalized polarizabilities $\alpha_n = \alpha/(\epsilon_e V)$ of regular polyhedra. Best numerical results according to [3]. The accuracy is such that the last number in the results for polyhedra should be correct to ± 1, except for tetrahedron in which case it is ± 5.

	polyhedron	$\alpha_n(\epsilon_r = \infty)$, PEC	$\alpha_n(\epsilon_r = 0)$, PEI
	tetrahedron	5.0285	-1.8063
	hexahedron	3.6442	-1.6383
	octahedron	3.5507	-1.5871
	dodecahedron	3.1779	-1.5422
	icosahedron	3.1304	-1.5236
	sphere	3	$-3/2$

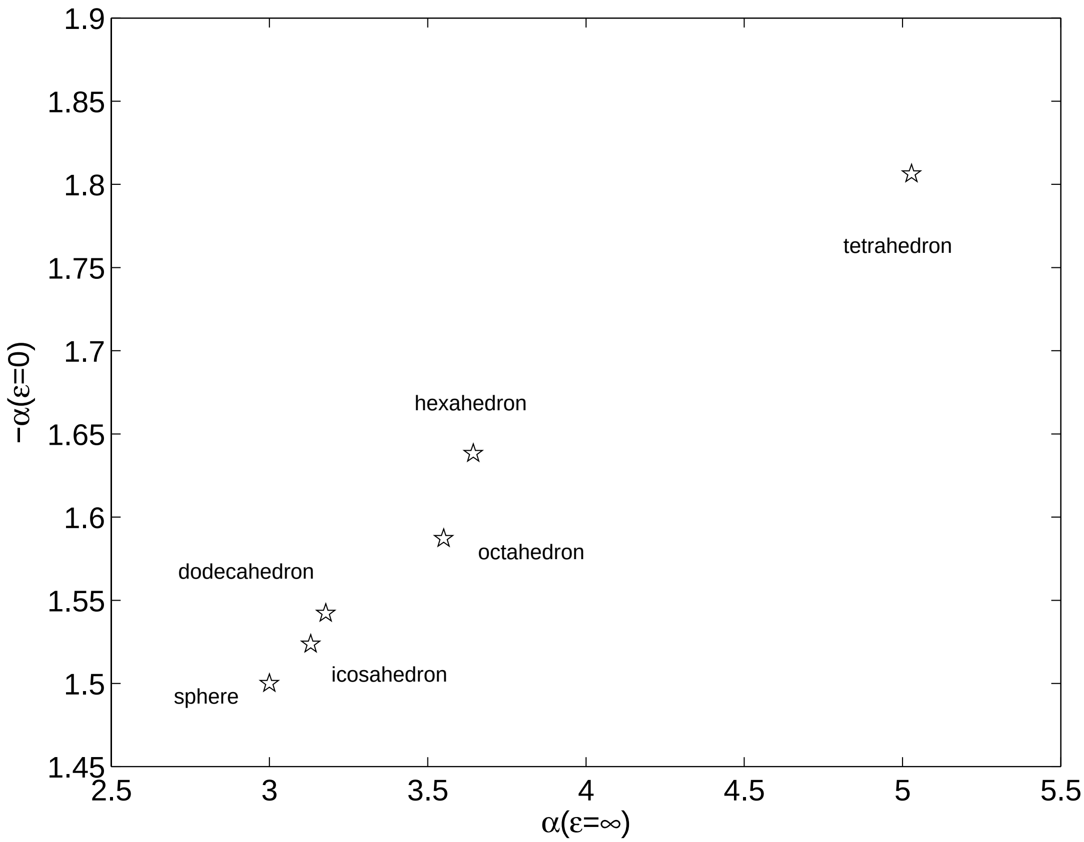


Figure 1: The polarizabilities of PEC and PEI inclusions against each other. The correlation coefficient of these two variables is 0.9901, meaning that the polarizabilities behave slightly differently for different polyhedra.

Table 2: Geometrical characteristics of polyhedra, with the corresponding parameters for a sphere.

polyhedron	faces	edges	vertices	solid angle seen from the vertex
tetrahedron	4	6	4	$3\arccos(1/3) - \pi \approx 0.55129$
hexahedron	6	12	8	$3\pi/2 - \pi \approx 1.5708$
octahedron	8	12	6	$4\arccos(-1/3) - 2\pi \approx 1.3593$
dodecahedron	12	30	20	$3\arccos(-1/\sqrt{5}) - \pi \approx 2.9617$
icosahedron	20	30	12	$5\arccos(-\sqrt{5}/3) - 3\pi \approx 2.6345$
sphere	∞	∞	∞	$2\pi \approx 6.2832$

Table 3: Additional geometric characteristics of polyhedra and the sphere. Note that the parameter a is the edge length (for the polyhedra) and radius (for the sphere) chosen with the requirement that the volume of the object be unity.

polyhedron	$a(V=1)$	specific surface	$R_{\mathrm{circ}}/r_{\mathrm{in}}$	g_{circ}	g_{in}
tetrahedron	2.039	7.20562	3	1.9359	1.5497
hexahedron	1	6.000	1.7321	1.3960	1.2407
octahedron	1.2849	5.71911	1.7321	1.4646	1.1826
dodecahedron	0.50722	5.31161	1.2584	1.1457	1.0984
icosahedron	0.771025	5.14835	1.2584	1.1821	1.0646
sphere	0.62035	4.83598	1	1	1

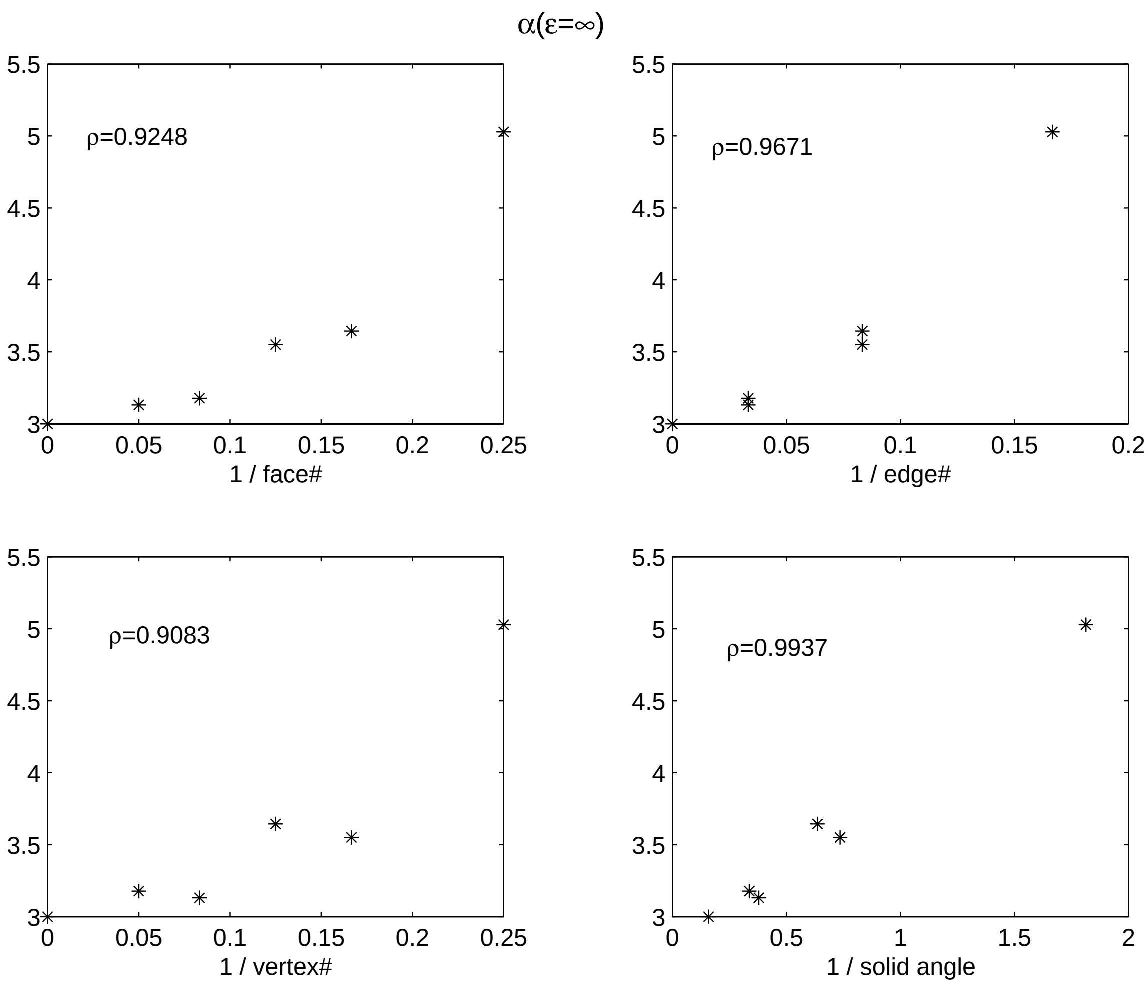


Figure 2: The polarizability of PEC inclusions and the geometrical parameters of Table 2.

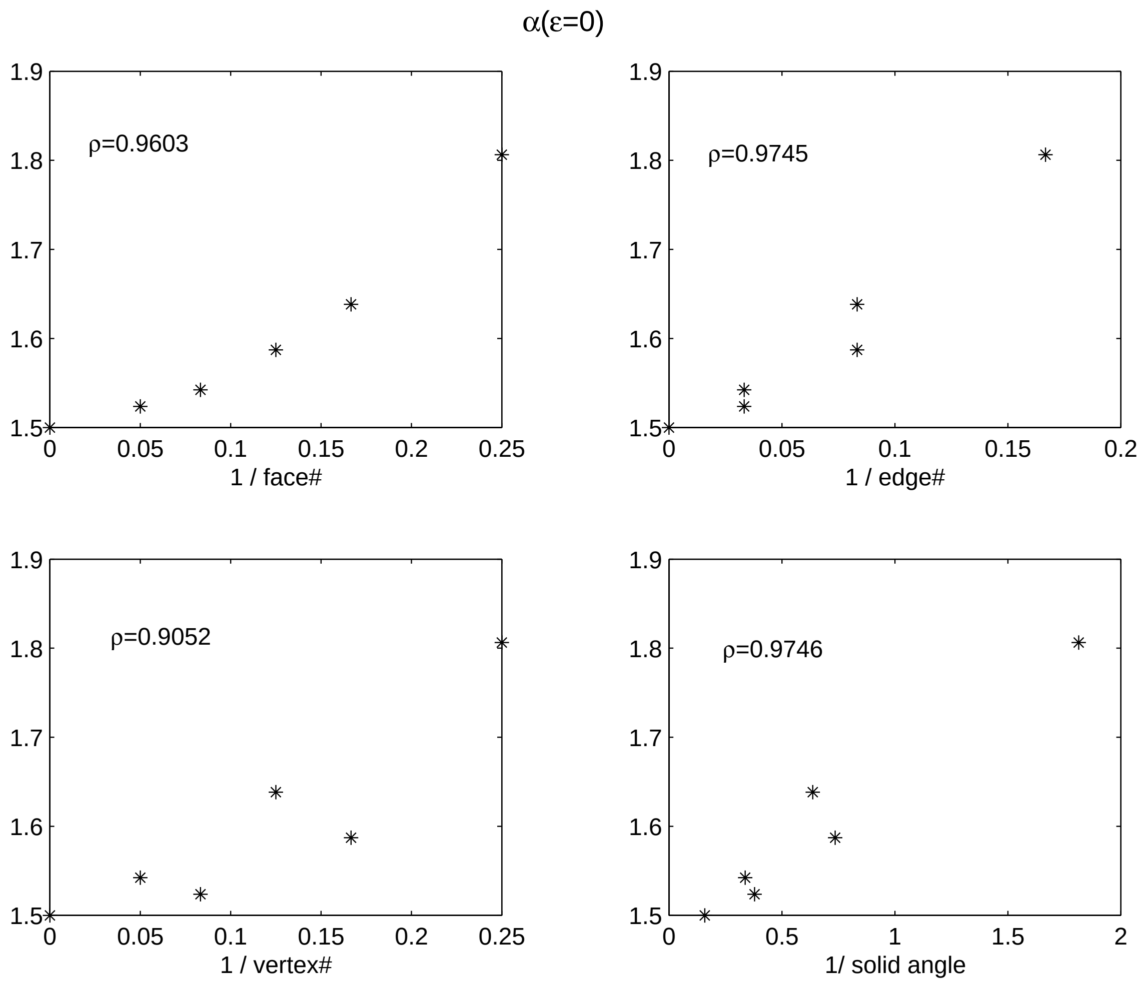


Figure 3: The polarizability of PEI inclusions and the geometrical parameters of Table 2.

Table 4: The correlation coefficients between the PEC and PEI polarizabilities with the geometrical parameters in Table 2.

	$\alpha(\epsilon = \infty)$	-$\alpha(\epsilon = 0)$	1/face#	1/edge#	1/vertex#	1/solid angle
$\alpha(\epsilon = \infty)$	1.0000	0.9901	0.9248	0.9671	0.9083	0.9937
-$\alpha(\epsilon = 0)$	0.9901	1.0000	0.9603	0.9745	0.9052	0.9746
1/face#	0.9248	0.9603	1.0000	0.9756	0.9278	0.9150
1/edge#	0.9671	0.9745	0.9756	1.0000	0.9756	0.9724
1/vertex#	0.9083	0.9052	0.9278	0.9756	1.0000	0.9359
1/solid angle	0.9937	0.9746	0.9150	0.9724	0.9359	1.0000

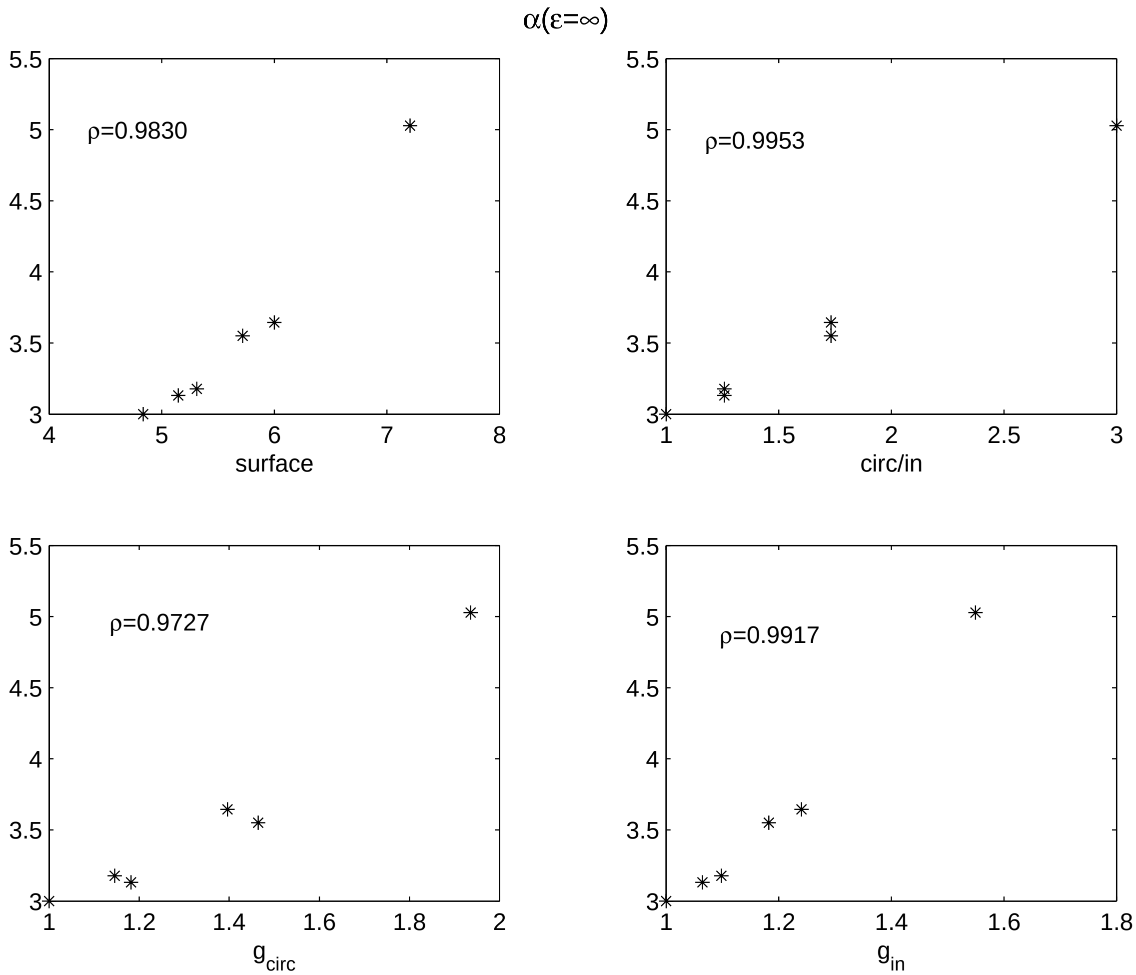


Figure 4: The polarizability of PEC inclusions and the geometrical parameters of Table 3.

Table 5: The correlation coefficients between the PEC and PEI polarizabilities with the geometrical parameters in Table 3.

	$\alpha(\epsilon=\infty)$	-$\alpha(\epsilon=0)$	surface	$R_{\rm circ}/r_{\rm in}$	$g_{\rm circ}$	$g_{\rm in}$
$\alpha(\epsilon=\infty)$	1.0000	0.9901	0.9830	0.9953	0.9727	0.9917
-$\alpha(\epsilon=0)$	0.9901	1.0000	0.9957	0.9878	0.9677	0.9977
surface	0.9830	0.9957	1.0000	0.9892	0.9802	0.9982
$R_{\rm circ}/r_{\rm in}$	0.9953	0.9878	0.9892	1.0000	0.9904	0.9938
$g_{\rm circ}$	0.9727	0.9677	0.9802	0.9904	1.0000	0.9789
$g_{\rm in}$	0.9917	0.9977	0.9982	0.9938	0.9789	1.0000

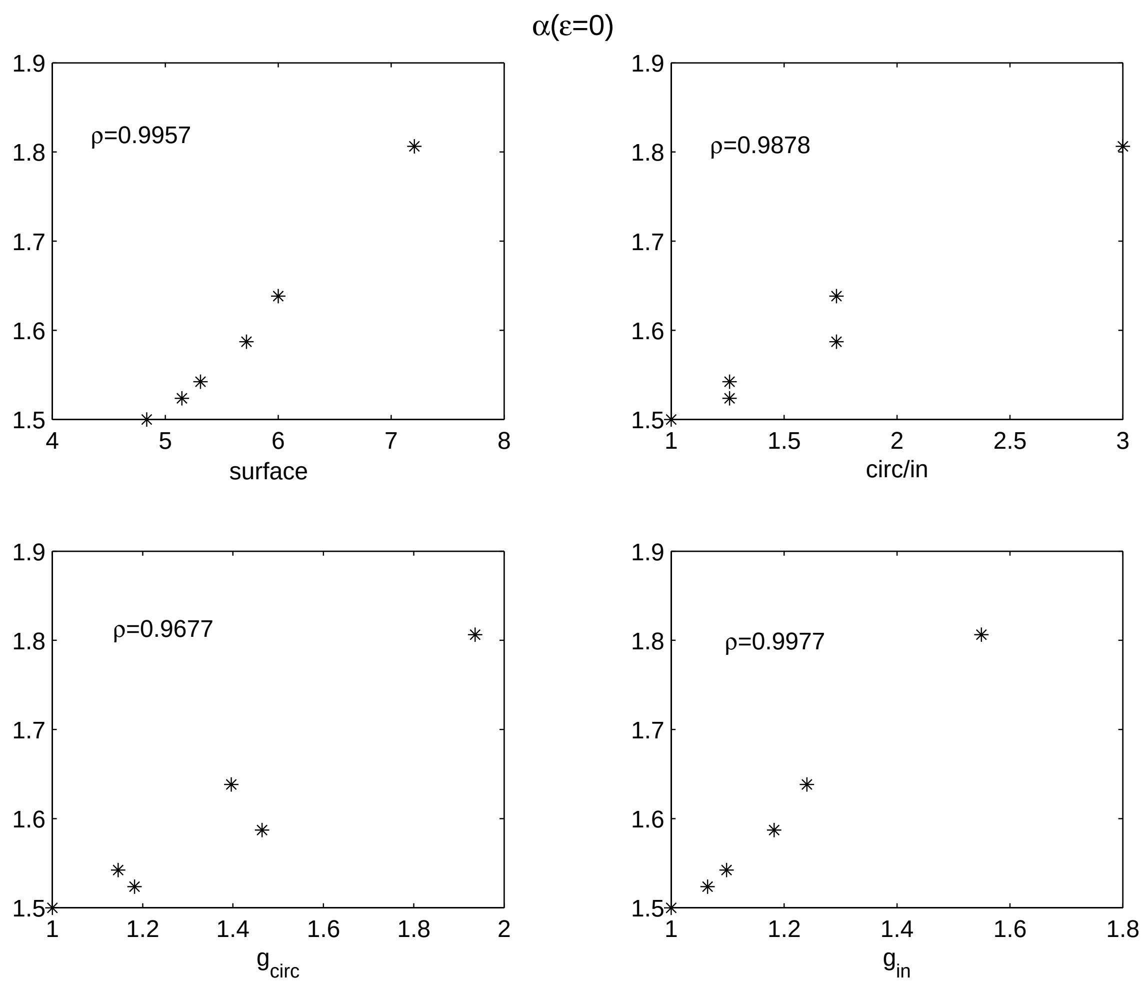


Figure 5: The polarizability of PEI inclusions and the geometrical parameters of Table 3.