Analytical solution of the depolarization field in biological objects of general shape

A. RAMÍREZ, L.R. DÍAZ, A. ZEHE,

Laboratorio de Nanotrónica, Facultad de Ciencias de la Electrónica
Benemérita Universidad Autónoma de Puebla,
Apdo. Post. #1505, 72000 Puebla, Pue.
MEXICO

Abstract: The dielectric response of biological cells is usually studied by measuring the impedance of suspensions or by a variety of single particle methods, that exploit different force effects. For biological objects the most striking frequency-dependent changes in polarizability result from structural (Maxwell-Wagner) polarization phenomena. Standard dielectric models consider the structural properties of cells by assuming spherical or ellipsoidal geometries. However, many such biological particles deviate from the ellipsoidal form. In the present paper an approximation procedure is derived for the general case of an arbitrarily shaped dielectric object. The here presented approach results in closed analytical solutions.

Key words: Bioimpedance, cell polarization, internal field.

1. Introduction

Microdevices for applications in a wide range of biologically and medically related technologies are increasingly based on the advanced technologies of microelectronic structuring and fabrication. Bioparticles are suspended in a stationary fluid, and force effects are imparted on them by the application of electric fields for dielectric characterization, trapping, manipulation or separation [1- 6]. Calculations of the frequency dependence of force effects are primarily based on spherical or ellipsoidal models, the standard approach to biological cells. In particular, single-shell models with Maxwell’s stress tensor [7] or the Laplace equation are used. In order to arrive at explicit solutions of the Laplace equation, a homogeneous ellipsoid as the only material body with a constant local (internal) field has to be assumed. Integrating over this field leads to the induced dipole moment, providing the exposure of the ellipsoid to a homogeneous external field. The induced dipole moment is directly related to force effects acting on the particle. How exact the frequency-dependent force effects and corresponding spectra can be reproduced, depends on the precision of the calculus for the local field and the dipole moment.

However, many particles and biological cells, including erythrocyte cell aggregates, as an example, deviate from the ellipsoidal form, and in order to account for these specially shaped cells, more adequate models are required.

Driven by the growing interest and impact of physical contributions to life sciences [8], complex geometries, such as rods and cylinders, need to be considered. Characterized by the unavailability of analytical solutions for the field distribution within such dielectric bodies, finite element numerical techniques have been developed recently [9], with the compromise of claiming considerable computer resources, though.

This paper deals with an approximation procedure for the calculation of the depolarization field $\vec{E_i}(\vec{r})$ in a material body of general shape, e.g. a 'coin stack' of erythrocytes, with a dielectric constant κ, which is brought into any given field $\vec{E_0}(\vec{r})$, yielding an analytical solution.

2. Depolarization field calculation

The problem, which is treated here, can be formulated as follows: The internal field $\vec{E_i}(\vec{r})$ generates a polarization.
This polarization induces on the surface element $\Delta\vec{F}$ of the dielectric body a polarization charge

$$\Delta q = \sigma_{pol} \cdot \Delta F = \vec{P} \cdot \Delta\vec{F},$$

which by virtue of the Coulomb law, together with the unperturbed field $\vec{E_0}(\vec{r})$, generates finally the depolarization field, such that

(1)

$$\vec{E}_i(\vec{r}_1) = \vec{E}_0(\vec{r}_1) - \oiint \frac{\vec{r}_{12}}{4\pi\varepsilon_0 r_{12}^3} [\vec{P}(\vec{r}_2) \cdot \Delta\vec{F}_2]$$

The integration is carried out over the surface of the dielectric body; $\Delta\vec{F}$ points outward, and $\vec{r}_{12}$ combines the origin at $\vec{r}_1$ with the integration element at $\vec{r}_2$. The relation between $\vec{E_0}(\vec{r})$ and $\vec{E_i}(\vec{r})$ is supposed by us to be lineal:

(2)

$$\vec{P}(\vec{r}) = \varepsilon_0(\kappa - 1)\, \vec{E}_i(\vec{r}) = \varepsilon_0(\kappa - 1)\alpha(\vec{r})\, \vec{E}_0(\vec{r})$$

In general, $\alpha(\vec{r})$ is a tensor, as the directions of $\vec{E}_i$ and $\vec{E}_0$ are not necessarily parallel. It further depends on the coordinates inside the sample due to the locally different action of the polarization charges. In order to calculate $\vec{P}(\vec{r})$ or $\vec{E}_i(\vec{r})$ from Eqs. (1, 2), we make the assumption, that α does not depend on $\vec{r}$, which of course is exactly fulfilled only in homogeneous ellipsoids. Here it is an approximation, which allows us to get to viable solutions which will be tested at the end by an experimental comparison.

The polarization, established inside the dielectric, is due to the displacement of the electrical charges enforced by the field $\vec{E_0}(\vec{r})$. Surface charges are built up and counteract the complete displacement corresponding to the field $\vec{E_0}(\vec{r})$. We will suppose here, that the whole set of charges experiences the same displacement, which means, that α=constant. We further suppose, that the polarization vector $\vec{P}$ points more or less into the direction of $\vec{E_0}(\vec{r})$, i.e., we will consider the projection of the field, generated by the polarization charges, on the direction of $\vec{E_0}(\vec{r})$:

(3)

$$\vec{P}(\vec{r}) = \varepsilon_0(\kappa - 1)\alpha_1 \vec{E}_0(\vec{r}_1)$$

$$= \varepsilon_0(\kappa - 1)\left\{\vec{E}_0(\vec{r}_1) - \oiint \frac{(\kappa - 1)\alpha_1}{4\pi} \cdot \frac{\vec{E}_0(\vec{r}_2) \cdot d\vec{F}_2}{\vec{r}_{12}^3} \cdot \frac{\vec{E}_0(\vec{r}_1) \cdot \vec{r}_{12}}{\vec{E}_0^2(\vec{r}_1)} \cdot \vec{E}_0(\vec{r}_1)\right\},$$

$$\alpha_1 = \left\{1 + \frac{\kappa - 1}{4\pi} \oiint \frac{(\vec{E}_0(\vec{r}_2) \cdot d\vec{F}_2)}{\vec{r}_{12}^3} \cdot \frac{(\vec{E}_0(\vec{r}_1) \cdot \vec{r}_{12})}{\vec{E}_0^2(\vec{r}_1)}\right\}$$

This value α_1 allows considering a first approximation of the polarization $\vec{P}_1$, which on the surface of the dielectric generates charges, and thus an additional field inside the dielectric. The problem would be completely solved, if the total field at any place fulfills already the condition

$$\vec{E}_i = \vec{P}_1 / \varepsilon_0(\kappa - 1)$$

but in general, the polarization $\vec{P}_1$ of the first approximation step will not be sufficient to describe the real situation, and a field $\vec{E_1}(\vec{r})$ keeps acting on the dielectric with the effect of an additional polarization $\vec{P}_2(\vec{r})$,

(4)

$$\vec{E}_1(\vec{r}) = \vec{E}_0(\vec{r}) - \oiint \frac{\vec{r}_{12}}{4\pi\varepsilon_0 r_{12}^3} (\vec{P}_1(\vec{r}_2) \cdot d\vec{F}_2)$$
$$- \vec{P}_1(\vec{r}_1) / \varepsilon_0(\kappa - 1)$$

$\vec{P}_2(\vec{r})$ can be calculated with $\vec{E_1}(\vec{r})$ in the same way, as $\vec{P}_1(\vec{r})$ was calculated with $\vec{E_0}(\vec{r})$.

The number of approximation steps needed to achieve the best results depends on the complexity of the shape of the dielectric body, as well as the allowed error of the result.

3. The depolarization field inside a cylinder shaped particle

Exact solutions are known for the sphere, the infinitesimal thin wire, and the infinitesimal extended disk. When our approach is applied here, already the first approximation step gives the exact solution, as it should be, when

$\propto(\vec{r}) = \propto_1 = constant.$

The polarization of a prolate spheroid (Fig. 1) results with Eq. 2 in

$$\propto = \left\{1 - (\kappa - 1) q^2 \left(1 + \frac{\sqrt{q^2+1}}{2} \cdot \ln \frac{\sqrt{q^2+1}-1}{\sqrt{q^2+1}+1}\right)\right\}^{-1}, \tag{5}$$

where $q = b^2/(a^2 + b^2)$.
For an oblate ellipsoid one gets

$$\propto = \left\{1 - (\kappa - 1)(q^2 + 1)\left(q \; arc \tan \frac{1}{q} - 1\right)\right\}^{-1}$$

and consequently with q → ∞ (or a = b) we have for the sphere-shaped dielectric $\propto = 3/(\kappa + 2)$ and thus the known result

$$\vec{P} = 3\varepsilon_0 \frac{(\kappa - 1)}{(\kappa + 2)} \cdot \vec{E}_0.$$

Not so straightforward is the situation in the case of a cylinder in a homogeneous electric field $\vec{E_0}(\vec{r})$ (see Fig. 2).
We get

$$\oiint \frac{E_0(\vec{r}_2)\cdot dF_2}{\vec{r}_{12}^{\,3}} \frac{\vec{E}_0(\vec{r}_1)\cdot \vec{r}_{12}}{\vec{E}_0^{\,2}(\vec{r}_1)} = 2\int_0^R \frac{2\pi a\, da \cdot L}{(a^2 + L^2)^{3/2}} \tag{6}$$

$$= \int_L^{(R^2+L^2)^{1/2}} \frac{r\,dr}{r^3} \cdot 4\pi L = 4\pi\left[1 - (1 + R^2/L^2)^{-1/2}\right]$$

$$\vec{P}_1 = \frac{\varepsilon_0(\kappa - 1)\vec{E}_0}{1 + (\kappa - 1)(1 - (1 + R^2/L^2)^{-1/2})}$$

Such a homogeneous polarization is only the first approximation. Due to the choice of the origin at z = 0, the by P generated field will be too weak in the transversal plane at z = 0, but along the z-axis at the limiting faces of the cylinder it is too strong. A field $\vec{E_1}(\vec{r})$ remains as given in Eq. (4), which delivers the depolarization at the cylinder top and bottom faces in a second approximation step.

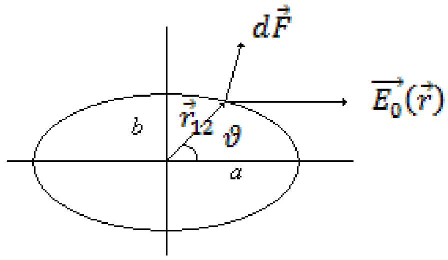

Fig. 1. Prolate ellipsoid

The integrations, involved in this step, are quite tedious and will not be carried out exactly here. We proceed instead as follows: $\vec{E_1}(\vec{r})$ is largest at the center of the plane cylinder faces, thus we put the origin $\vec{r}_1$ at the center of one of this faces S (see Fig. 2) and concentrate all the charge $\sigma_1 = |\vec{P}_1|$ at this center. (The real $\vec{E_1}$ migth be slightly larger, but this effect is compensated by a stronger inclination against the surface). The charge at the opposite side face acts on $\vec{r_1}$ after the Coulomb law, and provided L/R ≫1, like an point charge $\pi R^2 \sigma_1 / 4\pi\varepsilon_0 \cdot 4L^2$, but for L/R ≫1 like an extended charged disk with $\sigma_1/2\varepsilon_0$. A suitable interpolation or this field for the complete range L/R is about $(\sigma_1/2\varepsilon_0)(1 + 8L^2/R^2)^{-1}$. The normal component of field belonging to the side face, which contains $\vec{r_1}$ is $\sigma_1/2\varepsilon_0$, and consequently results the normal component $\vec{E_1} \perp s$ at both side faces S to

$$\vec{E}_{1\perp s} = E_0 - \frac{\sigma_1}{2\varepsilon_0} - \frac{\sigma_1}{2\varepsilon_0}(1 + 8L^2/R^2)^{-1} - \left(\frac{\sigma_1}{\varepsilon_0(\kappa - 1)}\right)$$

The normal component of $\vec{E_1}$ at the cylinder cover area C (see Fig. 2) is approximately

$$\vec{E}_{1\perp C} = \frac{\pi R^2 \sigma_1 \cdot R}{4\pi\varepsilon_0[R^2 + (L - z)^2]^{3/2}} - \frac{\pi R^2 \sigma_1 \cdot R}{4\pi\varepsilon_0[R^2 + (L + z)^2]^{3/2}}$$

The surface integral of α_2 contains then the following contributions: 2π from the top faces containing $\vec{r}_1$, $2\pi\left[1-(1+R^2/4L^2)^{1/2}\right]$ from the opposite side face, and from the cover area C

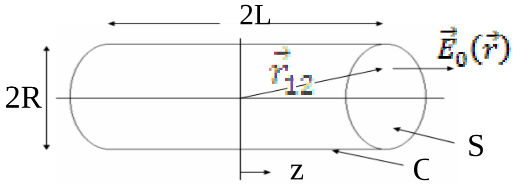

Fig. 2. Dielectric cylinder of length 2L and diameter 2R.

$$\frac{R^3}{4}\left[\frac{\varepsilon_0}{\sigma_1}-\frac{1}{2}-\frac{1}{2}\left(1+\frac{8L^2}{R^2}\right)^{-1}-\frac{1}{\kappa-1}\right]^{-1}$$

$$\times\int_{-L}^{L}\frac{2\pi R(L-z)dz}{[R^2+(L-z)^2]^{3/2}}$$

$$\times\{[R^2+(L-z)^2]^{-3/2}-[R^2+(L+z)^2]^{-3/2}\}$$

Thus

$$\alpha_2=\left\{1+(\kappa-1)\left[1-\frac{7}{16}(1+11R^2/56L^2)^{-1}\right]\right\}^{-1}$$

The surface charge density $\sigma_2=\varepsilon_0(\kappa-1)\alpha_2\vec{E}_1\perp$ when added to σ_1 has the effect of reducing the density of the side faces, but increasing it on the cover area close to the side faces. The dipole moment of the cylinder in a second approximation yields then

$$\vec{p}=\pi R^2\varepsilon_0(\kappa-1)\left\{1+(\kappa-1)\left[1-(1+R^2/L^2)^{-\frac{1}{2}}\right]\right\}^{-1}\vec{E}_0$$
$$\times\left\{2L+\frac{L-2L(1+R^2/L^2)^{-1/2}-L(1+8L^2/R^2)^{-1}+(R^2+2L^2)\cdot(R^2+4L^2)^{-\frac{1}{2}}-R}{(\kappa-1)^{-1}+1-7/16(1+11R^2/56L^2)}\right\}. \quad (7)$$

The first part of the equation describes a homogeneous polarization under consideration of only the charge density situated on the side faces *S*, and the remaining part considers, as a second approximation, a slight depolarization contribution at both ends of the cylinder.

4. Conclusion

The general approach for the calculation of the depolarization field in biological objects (or particles of any shape) is exemplified by the derivation of an analytical expression for the dipole moment of a short cylinder shaped particle (e.g. a stack of erythrocytes). The second approximation counts for about 10% improvement of the otherwise obtained result under consideration of a homogeneous polarization alone.

Acknowledgement

Financial support of VIEP, B. Universidad Autónoma de Puebla México, under proyect # 17/ING/06-G is gratefully acknowledged. The authors thank María del Carmen Ramírez D. for help in the manuscript preparation.

References

[1] Pauly H & Schwan HP (1959). *Zeitschrift für Naturtorschg*, 14b: 125-131.
[2] Asami K, Hanai T & Koizumi N (1980). *Jap. J. Appl. Phys.*, 19:359-365.
[3] Griffin JL (1970). *Exp.l Cell Res.*, 61: 113-120.
[4] Miller RD, Jones TB (1993). *Biophys.J*, 64:1588
[5] Zimmermann U & Neil GA (Editors), *Electromanipulation of Cells.* CRC Press, Boca Raton, N.Y., London, Tokyo (1996).
[6] Stoylov SP (1996). *Biophys. Chem*, 58: 165-172.
[7] Wang X, Wang XB & Gascoyne PRC (1997). *Journal or Electrostatics*, 39:277-295.
[8] Kotnik,T, D.Miklavcic (2000). *Biophys. J*. 79 670.
[9] J. L. Sebastián, S. Muños, M. Sancho, J. Miranda (2001). *Phys. Med. Biol.* 46 213-221