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Fractal frontiers in microelectronic ceramic materials

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Abstract:

The world's perennial need for energy and microelectronic miniaturization brings with it a broad set of technological and scientific challenges. Materials characterized by precise microstructural architectures based on fractal analysis and ranging in size down to nano scale represent an important avenue for finding novel solutions. Deep materials structure hierarchies of this type open new possibilities in capacity according to the Heywang model, especially when extended by a fractals approach and intergranular relationships supported and recognized by their fractal nature. These developments are opening new frontiers in microelectronics miniaturization. They build on early fractal applications that were used as tools in miniaturization research and also provided application perspectives for diverse energy technologies. In other words, fractals, as a crucial concept of modern theoretical-experimental physics and materials sciences, are tightly linked to higher integration processes and microelectronics miniaturization. They also hold potential for meeting the energy exploitation challenge. In this research context, for the first time we

experimentally and theoretically investigated the electrostatic field between the grains within fractal nature aspects. It is essentially a theoretical experiment based on samples of experimental microstructures imaged with SEM, as previously published in a number of other papers. We now take the research a step further by consolidating the experimental samples with respect to the predicted distribution of grains and pores within the sample mass.

We make an original contribution by opening the frame of scale sizes with respect to the technical processes of consolidation. This lets us predict the constitutive elements of the microstructures – approximately equidistant grains and pores. In this paper we define in a practical manner the final target elements for experimental consolidation of real samples. It is the main bridge between a designed microstructure and related characteristics – for example, fractal dimensions and final properties of next-generation fractal microelectronics.

Key words: Ceramic materials, microelectronic miniaturization, fractals, electrostatic field, energy technologies

1. Introduction

Developing the technological processes and methods for designing real ceramics is vital for producing materials samples with fully-controlled grains, pores and the bi-layers in between them that constitute the ceramic structures. Controlling the distribution of grains and pores and the thickness of the layers separating them opens perspectives on completely new approaches to, and areas of, miniaturized microelectronics and high-level multifunction integrations. It means that in these media we can see the parameters for future electronic integrations within the fractal electronics framework of intergranular fractals phenomena. Using fractal analysis and calculations we can provide the geometric, design and other parameters for these new technological processes necessary for exploiting the new frontier in sample synthesis.

Fractal analysis provides the requisite microstructure dimensions which are crucial for designing the experimental samples consolidation parameters. We are practically at the point where we can begin to plan real experiments on the way to developing the samples. Accordingly, in this paper we predict the parameters for a real experimental procedure. This is not as easy an endeavor as when semiconductor technology applications were first developed.

Simply confirming that there exist minimum possibilities for continuing along fractals perspectives combined with new technological methods could constitute a technological processing breakthrough.

As such, continuing the research on the fractal structure nature of ceramics and materials in general will have a significant impact on completing the super micro capacitor – its capacity and fractals microelectronics frame.

Hence, in this research paper we complete the previously developed structural and technological tools and integrate them with recent findings on the consolidation of materials, especially ceramics. The focus is on electro/electronic ceramic materials, designing electrostatic field allocations, and an initial procedure for defining the dimensions of contact surfaces and bi-layer coating films between grains in light of fractal characterization. All of these scientific goals include fractal nature relativization on the microstructure morphology scale: mega-meso-micro-nano.

In general, the fractal nature analysis approach is key for work on all future new materials frontiers, for example as in miniaturization and developing alternative energy sources. In fact, we are analyzing microstructure from a real experimental procedural perspective and collecting all necessary parameters for fractal corrections.

This research is framed by the goal of advancing microelectronics miniaturization and micro packaging on the cutting edge of fractals microelectronics. In addition, we seek to define the possibilities for correlating electrostatic super micro intergranular capacitors and micro electrostatic fields on the one hand and energy and energy storage with materials of a fractals nature in general on the other, [1-9].

1. Introduction to fractals

Here we will discuss the role fractal geometry and analysis play in answering questions on microstructures at all levels of technology ranging from the mega to the nano scale. as well as on miniaturization and energy as a property of physical objects which also exhibit some features characteristic of fractal objects.

Fractals are geometric objects with broken, fragmented, wrinkled or amorphous forms or that are highly irregular in some other way. Euclid's standard geometry fails to describe such objects; instead, they must be studied with fractal geometry. "Fractal" was a neologism derived by Mandelbrot [10] from the Latin adjective *fractus*, meaning "fragmented, irregular".

Many fractals possess strict geometric self-similarity: they are invariant under any transformation of similarity (homothety) like a Cantor set, Koch snowflake, Sierpinski triangle, Conway triangle (Fig. 1a) or Menger sponge, etc. But many more consist of parts that resemble the whole in some other way. At times, the resemblance may be only approximate or statistical (Mandelbrot set, Julia sets). Unlike these ideal (mathematical) fractals, physical (real) fractals (Fig. 1b) closely approximate their ideal counterparts and are called pre-fractals (or proto-fractals); typical examples include trees, forests, earth relief, micro-particles, and labyrinths of pores in porous materials, etc.

It is clear that self-similarity, which is equivalent to scale invariance, is a direct consequence of contractive (or dilation) symmetry [12]. The usual definition of symmetry assumes that for a symmetric object S there exists transformation T so that – provided T has unit norm – T does not change the size of the object, just transforms

the object inside itself. On the other hand, for fractal object S , there exists transformation T that satisfies

$$\|T\| < 1, \text{ and } T(S) = S.$$

In this case, T is called transformation of dilation symmetry.

Fig. 1. The Richardson-Mandelbrot diagram for: a. Mathematical fractal (Conway triangle, $D_H \approx 1.7227$); b. Real fractal - the SE microphotograph of BaTiO_3 ceramics doped by 0.1 wt% of Holmium (Ho_2O_3). Fractal dimensions differ in different ranges of magnitude, as expected from real fractals (pre-fractals).

Fractal objects can be classified by their fractal dimension as *fractal dots* (usually called fractal dust) with $0 < D_H < 1$ (ex.: Cantor set,), *fractal lines* with $1 < D_H < 2$ (ex.: Koch snowflake, [10]), and *fractal surfaces* with $2 < D_H < 3$ (ex.: Menger sponge), etc. ([11], [13-26]).

2. The experiment

BaTiO_3 -ceramics and others are very “exciting” and highly advanced materials used in current research that have seen sustained growth in a variety of applications (over 300 different ones have been developed to date).

We prepared our research samples using a conventional solid state sintering process starting from reagent-grade powdered BaTiO_3 (Murata, Rhone Poulenc $\text{Ba/Ti}=0.996\pm 0.004$) doped with these additives: CeO_2 , Bi_2O_3 , Fe_2O_3 , MnCO_3 , CaZr_2O_7 , Nb_2O_5 , Er_2O_3 , Yb_2O_3 , Ho_2O_3 , La_2O_3 , Dy_2O_3 , and Sm_2O_3 . The additive content ranged from 0.01 to 1.0 wt%. Starting powders were ball milled in ethyl alcohol. After milling, the

powders were dried for several hours, then pressed into pellets 2 mm thick and 7 mm in diameter at a pressure ranging from 35 to 150 MPa. The pellets were sintered in air from 1180°C to 1380°C for 2 and 4 hours. The microstructure of BaTiO₃ doped samples was investigated with a JEOL SEM-5300 scanning electron microscope equipped with an EDS (Energy Dispersive Spectrometer) system. The electrical characteristics were measured using an Agilent 4284A LCR meter in a frequency range from 20 Hz to 1 MHz. Most microstructures were made from select grains and pores with a minimum of five magnifications, which is important for microstructure fractal nature analysis. [27-33]

We selected a typical microstructure for the sintering consolidation process, i.e., one where a "neck" connected the grains and there was a corresponding lacunar porosity SEM image (Fig. 2.). These microstructure morphologies are crucial for understanding and explaining micro intergranular capacity and general electro-physical characteristics, especially those influencing supermicro electro capacity and micro intergranular impedance. To obtain a more complete structure, we also applied fractal characterization.

Fig. 2. BaTiO₃-ceramics microphotograph, evidencing porous material within the viscous sintering process This corresponds to lacunar fractal models.

This yielded a new phenomenon, namely, that solidification increases overall fractal dimension. Thus emerged one more correction factor α .

2.1. The theoretical experiment

Based on the results of real microstructure consolidation we developed the approach which best explains the intergranular Heywang-model micro capacitors.

From that perspective, we illustrate it with a polyhedral-isohedral geometry morphology structure (Fig. 3.), with micro places corresponding to each other between two grains and responding to effects of a real electrostatic field on the micro level. For this purpose, we used a COMSOL software package specialized for electrostatic fields analysis of two particles/grains systems (Fig. 4., Fig. 5.) and for the five particles/grains system (Fig. 6.).

COMSOL is a finite element method software package for various physics and engineering applications, especially coupled phenomena or multiphysics. For simulation purposes, the AC/DC module is used with an “electrostatics” interface. The geometry of the fractals nature is modeled as spherical particles guided by illustrations . Thus, it is modelled with a domain whose dimensions are much greater than the dimensions of the fractals with boundary conditions set to zero potential. The problem of electromagnetic analysis on a macroscopic level requires solving Maxwell’s equations subject to certain boundary conditions. This set of equations written in differential or integral form describes the relationships between the following fundamental electromagnetic quantities:

- Electric field intensity E
- Electric displacement or electric flux density D
- Magnetic field intensity H
- Magnetic flux density B
- Current density J

- Electric charge density ρ

$$\nabla \times H = J + \partial D / \partial t$$

$$\nabla \times E = -\partial B / \partial t$$

$$\nabla \cdot D = \rho$$

$$\nabla \cdot B = 0$$

When using FEM analysis software, the key step is creating the mesh of elements before performing any computations. Using a finer mesh produces a greater number of elements and thus more accurate results. However, finer mesh requires more powerful hardware and longer computational time. It is essential to find the proper balance between result accuracy and time. For the analysis presented in this paper, we selected a free tetrahedral mesh featuring a corner refinement option. Fine adjustments in maximum and minimum element dimensions had to be made for each of the domains (fractals and surrounding soil domain).

Fig. 3. Illustrating the progressive evolution of grain boundary and pore structures associated with a single grain

For electrostatic field simulation-analysis of two-particles/grains systems we applied the following parameters : radii of particles/grains were 2μ , particle distance was 0.5μ , the charges per particles/grains were $1e$ for the left and $2e$ for

the right particle. For five-particle systems, we applied charges of $1e$, $-1e$, $2e$, $1e$, $-2e$ respectively, with the other parameters kept the same.

Fig. 4. electrostatic field distribution of two particles/grains

Fig. 5. Electrostatic field on an axis between two particles.

Fig. 5. shows the relationship between the electric field norm and arc length of an equiscalar field surface. According to the microstructure distances and electrostatic charges of the particles/ grains it is clear that arc lengths up to 0.16 parallel a decrease in the electrostatic field norm. However, from 0.16 to 0.3 we observed some slight growth in the electrostatic field norm followed by drastic electrostatic field norm growth.

Fig. 6. A field for a five-particle system

2.2. Particles/grains and electrostatic fields by the fractal nature approach

Based on our previous results, especially with respect to microstructure characterization, the grains and pores surfaces in complete ceramics morphology structures evidence a fractals nature [34,35]. After much experimentation, we succeeded in characterizing the surfaces of structure constituents like grains and pores. This confirmed the feasibility of reconstructing them using the fractal method

[36,37]. Therefore, we needed to define how the fractal nature influences the grain surfaces and thus the electrophysical properties characterizing the electrostatic field between two grains and within grain clusters. With that aim, we developed a MATLAB application for many microstructure experimental results (Fig. 7.) that recognizes the fractal surfaces of grains. Compared to results from grain surfaces defined by Euclidean geometry, which does not recognize their fractal nature (Section 2.1), reliance on fractal nature analysis produces more precise and more realistic hence satisfactory results. This stems from applying the fractal correction perspective to micro intergranular electrocapacity and other electrophysical characteristics like electrostatic fields. Here we apply the extended fractal-capacity Heywang model based on the Mitic-Kocic approach [38].

Fig. 7. Electrostatic field distribution of two particles/grains with recognized fractal nature surfaces

2.3. Results and discussion

Here we compare and discuss the results from fractal nature analysis of an idealized Euclidean geometry microstructure with morphology in BaTiO₃-ceramic structures.

The electric field of a conducting sphere with charge Q can be obtained by a straightforward application of Gauss' law. Considering a Gaussian surface in the form of a sphere at radius $r > R$, the electric field has the same magnitude at every point of

the surface and is directed outward. The electric flux is then just the electric field multiplied by the spherical surface area. Using Gauss's law, the electric field of a point charge can be obtained.

$$\Phi = EA = E4\pi r^2 = \frac{Q}{\epsilon_0} \quad (2)$$

The electric field turns out to be identical to that of a point charge Q at the center of the sphere. Since all of the charge will reside on the conducting surface, a Gaussian surface at $r < R$ will enclose no charge, and due to its symmetry is observed to be zero at all points inside the spherical conductor.

$$E = \begin{cases} \frac{1}{4\pi\epsilon_0} \frac{Q}{r^2} & r > R \\ 0 & r \leq R \end{cases} \quad (3)$$

The electric field in a system with multiple point charges can be obtained by taking the vector sum of the electric fields of the individual charges.

Taking the Mitic-Kocic fractal approach to intergranular micro capacity by the Heywang model [39-41] we analyzed the fractal correction based on the results obtained in Section 2.2. Our fractal nature analysis carried out on micro intergranular capacity and the corresponding fractal correction α prior to this study was not a factor in any electrophysical equations defining the micro electrostatic field. As the intergranular capacity is based on the micro electrostatic field, extending fractal characterization to the level of the electrostatic field is acceptable. Equation (3) is modified by introducing a correction factor [42,43]

$$\alpha = (N\xi^2)^k \quad (4)$$

The correction factor is obtained by taking a constructive approach to the fractal sphere surface. This approach uses an algorithm that iterates N self-affine mappings with a constant contractive (Lipschitz) factor $|\xi| < 1$ k -times.

Finally, equation (3). reduces to:

$$E = \begin{cases} \frac{1}{4(N\xi^2)^k \pi \varepsilon_0} \frac{Q}{r^2} & r > R \\ 0 & r \leq R \end{cases} \quad (5)$$

Hence, in principle, including the fractal correction with values for the fractal surface that are higher than for a smooth Euclidean geometry surface resulted in correspondingly lower electric field values. This discussion leads us to conclude that it is possible to have electrostatic field parameter estimation that completes the extended Heywang intergranular capacity model as a fractal capacitor. Our research previously introduced fractal correction based on SEM-imaged microstructure geometric parameters that are pure experimental data. Furthermore, we performed the fractal correction as a complex fractal correction which recognizes the influence of grain and pore surfaces as well as the Brownian particles motion phenomena observed in real experimental electrophysics characterization and presented as an effect of three dimensional trajectory curvature. Hence, certain previous results are simply applied here as foundation for the fractal analysis and corrections implemented in this study. Given the state of miniaturization development today, new approaches and technologies are clearly needed if the field is to advance. Solutions proposed to date

do not answer this need. With our fractal analysis of the intergranular thin layers of contact surfaces we are creating new opportunities for leading-edge theoretical, experimental, and technological advances. Consequently, to better understand and control very subtle electrophysical laws and associated properties (R, L, C) we must furnish specific corrections for future research and calculations on these super micro fractal levels. This is critical for the future of fractal microelectronics. In future research, , instead of relying on “classic” semiconducting technologies, we see a need to search for new opportunities in semiconducting ceramics for electronics through more highly-integrated electronics properties.

By using parameters of micro dimensions in combination with this micro electrostatic field in the fractal nature frame, we can design cutting-edge BaTiO₃ samples or other ceramics with advanced predictable and controlled structures. It also creates the potential for prognosticating properties (R, C, L) in media between the grains in the perspective space (bi-layers) for higher integrations of microelectronics parameters in the fractal nature frame.

In the area of energy harvesting and storage, especially given what is happening with new alternative energy sources, new approaches are critical if we are to have more precise estimation of effective contact surfaces – precisely where we are introducing the approach of fractal nature analysis. We are convinced that fractals analysis yields higher energy storage values.

This calls for continued experimental development in designing, predicting, and prognosticating materials porosity and pores distribution, functional fractals capacity, and designing bi-layers between grains (i.e. thin-film grain coatings).

Conclusion

There can be no question that when it comes to further miniaturization potential, semiconductor technologies have nearly reached their limit. It is therefore vital that we create new methods and scientific tools based on fractal nature characterization for a novel approach to advanced microelectronic miniaturization. Moreover, given the fractal nature found in ceramics and in materials generally in all morphologies and structures, interfaces and layers in nature, we are pioneering a new fractal microelectronics in this paper.

Our having involved micro electrostatic fields between the grain clusters within fractal nature is a first for the material sciences. The difference that fractal correction on electrostatic fields makes as compared with experimental observations by Euclidean geometry is evident. We are pioneering the prediction of micro dimensions on grains in and between pores as well as the corresponding electrophysical parameters, which is the prerequisite for experimental advances in defined ceramics samples.

The next step in complex fractal characterization will require conducting realistic and theoretical physico-mathematical experiments. They hold the promise of advances in the following fields that will eventually lead to completely new aspects of miniaturizing integrated electronic parameters and advances in related technologies:

- Brownian motion in fractals nature,
- further analysis of mutual distribution of fractals correction influence based on grains surface and pores,
- analysis and influence on process control in supermicro-nano contacts of grains and pores surfaces,
- fractals correction influence on micro capacity
- contribution of fractals correction to further improvement of intergranular Heywang capacity model,

These results also open the way to new approaches for more precisely estimating effective contact surfaces through fractal nature analysis that will result in contact surfaces with higher energy storage values. This, too, offers a radically new perspective and thinking on the energy harvesting and storage field.

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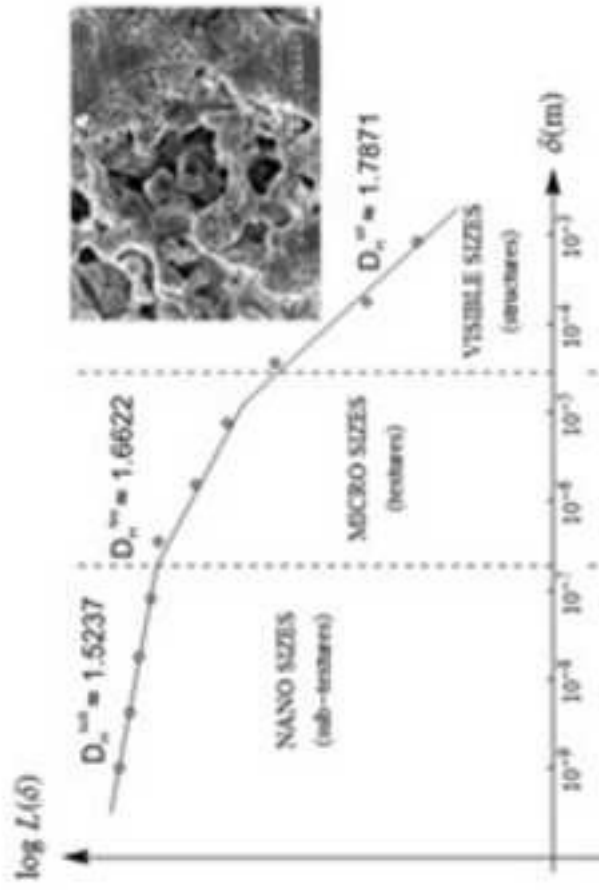
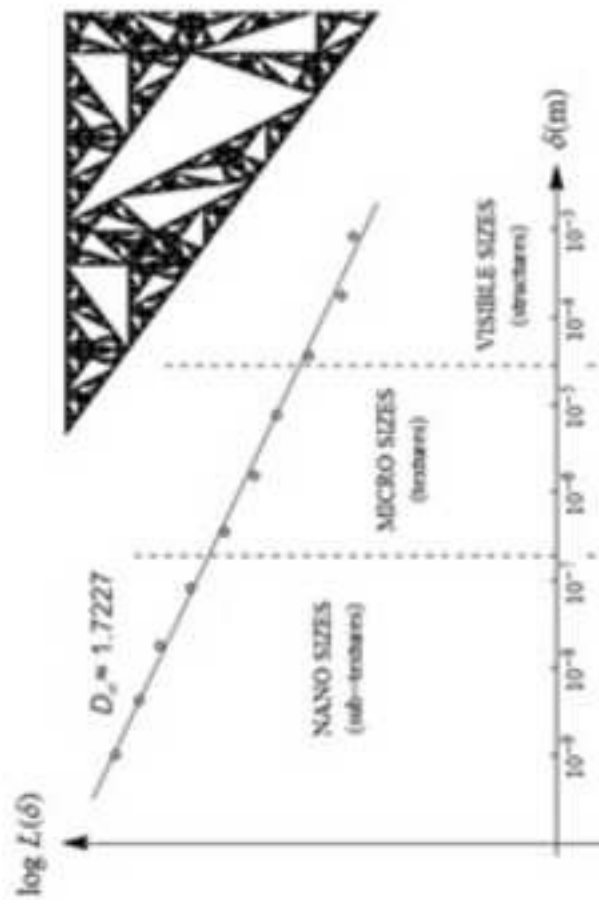
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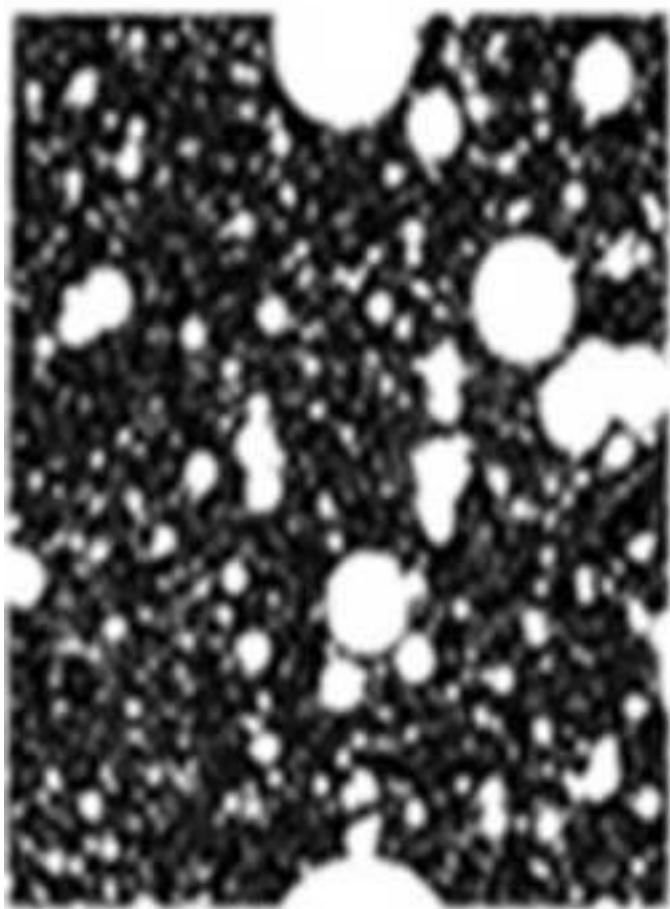
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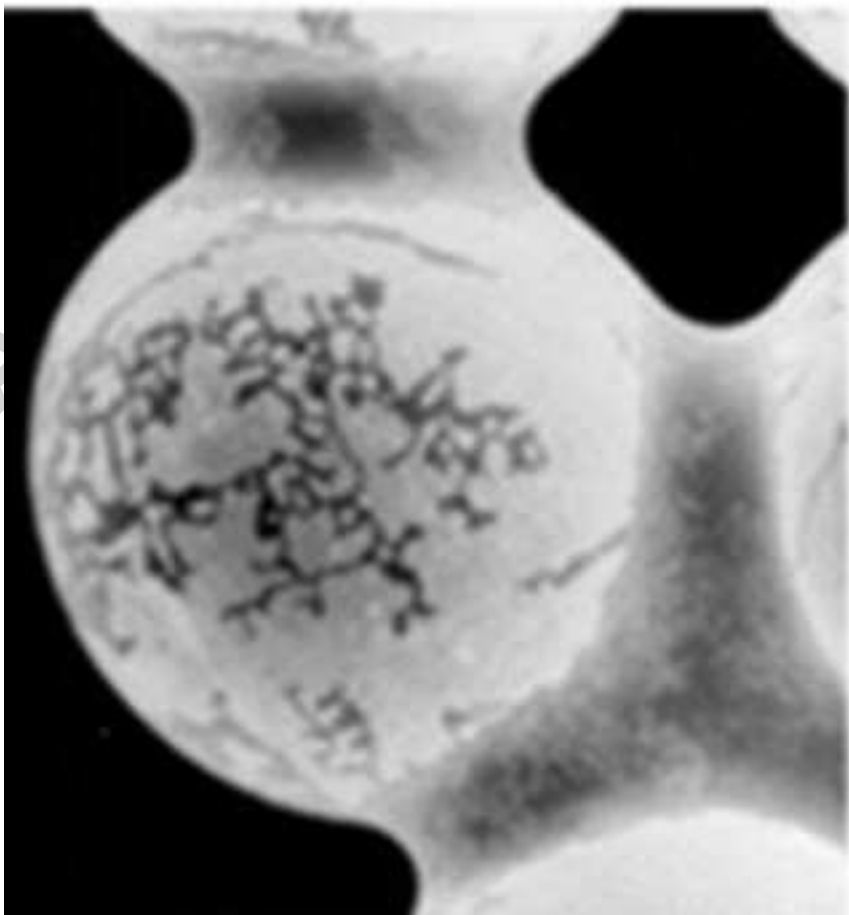
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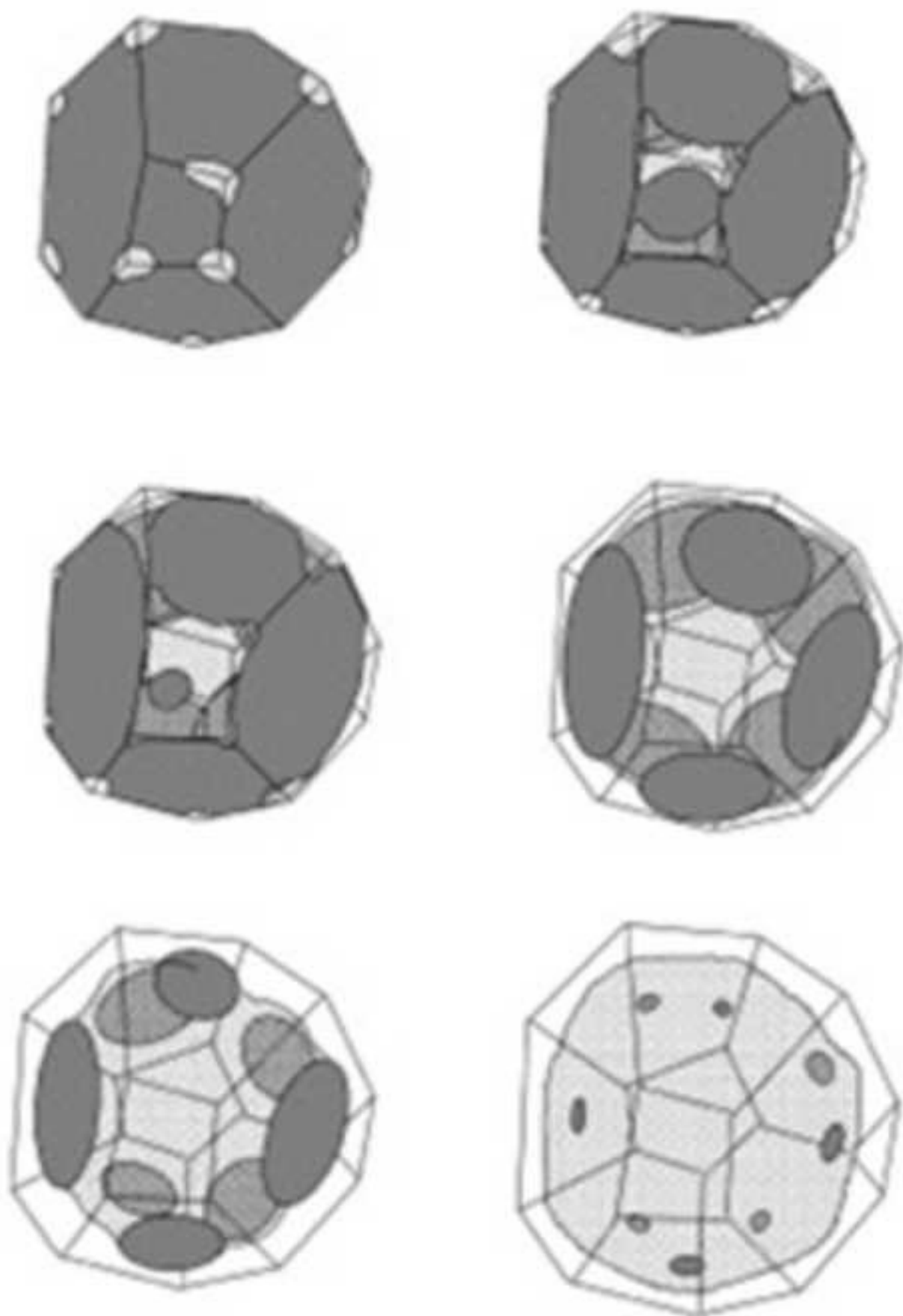


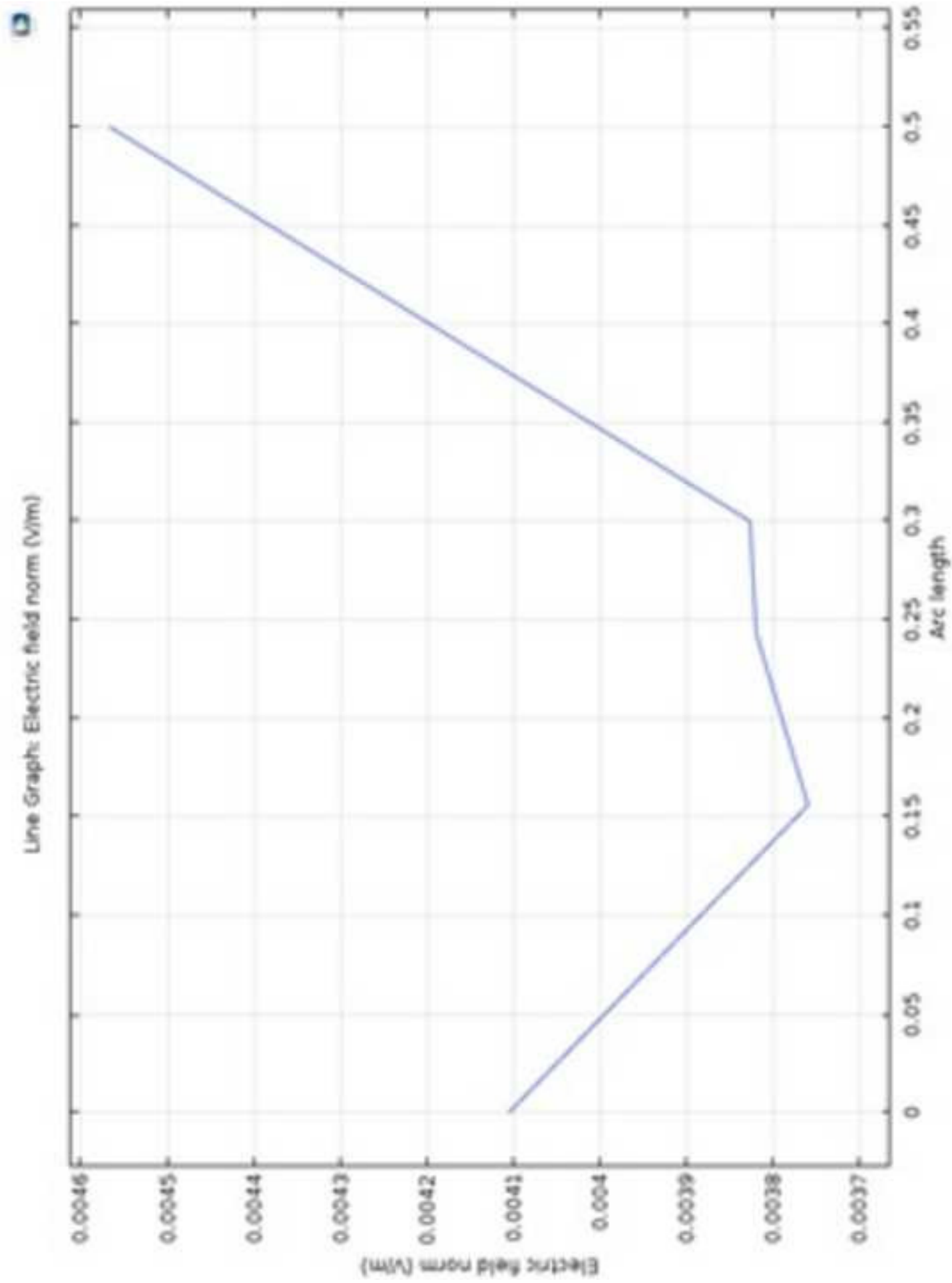
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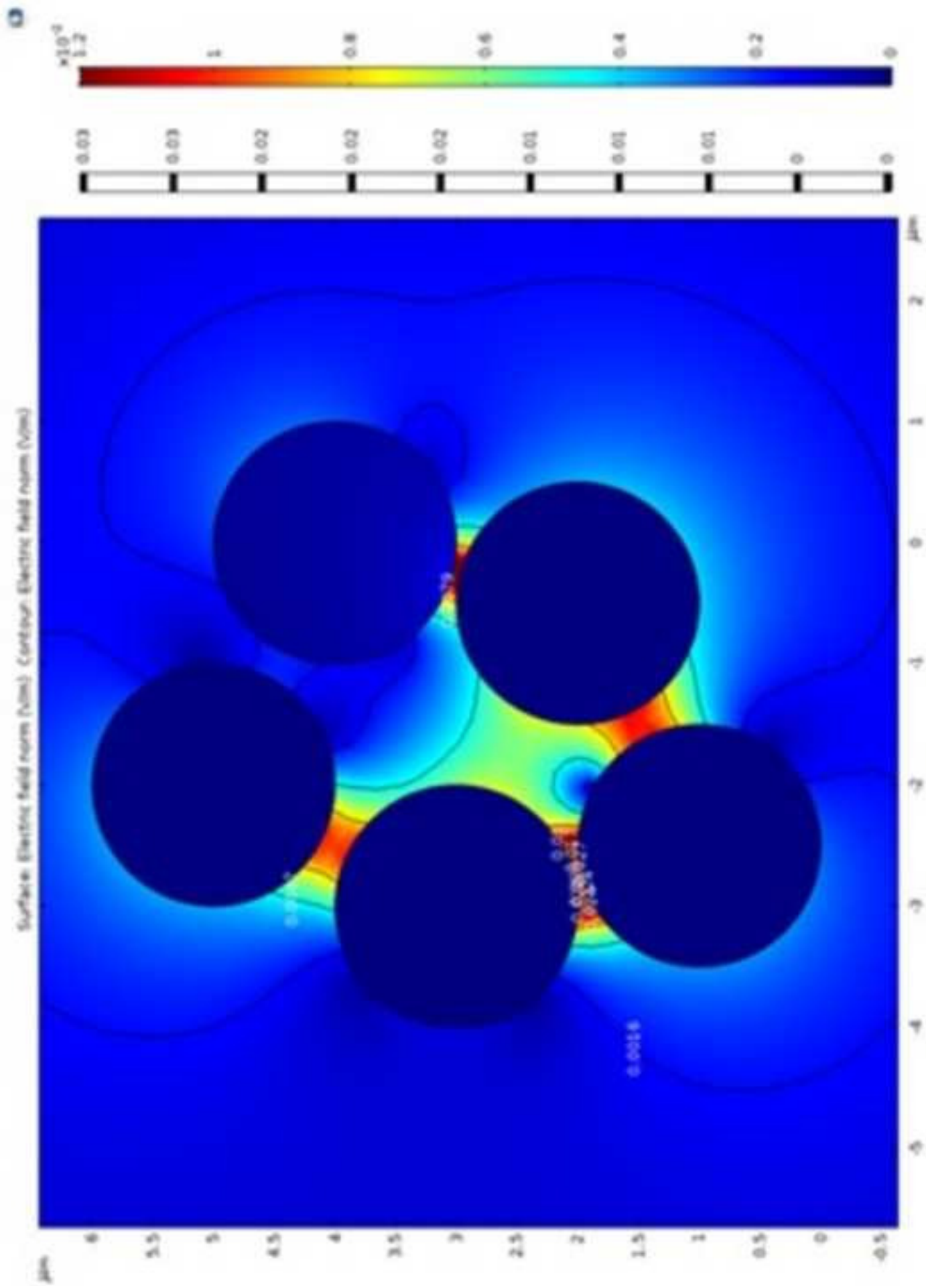


$$D \approx 2.75$$









Figure

