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Influence of electrode geometry on growth of horizontally aligned carbon nanotubes

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Abstract. This work investigates the influence of electrode geometrical parameters on the electric-field-strength distribution required for the directed growth of horizontally aligned carbon nanotubes by plasma-enhanced chemical vapor deposition. Optimal electrode parameters that provide maximal electric field strength and high efficiency of aligned nanotube growth have been determined. The influence of electrode shape (rectangular, semicircular, and triangular) on the field-strength distribution and nanotube alignment is demonstrated. The results contribute to optimizing the growth process of horizontally aligned carbon nanotubes for applications in sensors and nanopiezotronic devices.

Keywords: carbon nanotubes, horizontal growth, PECVD, electric field, electrode, modelling, directed growth

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Влияние геометрии электрода на рост горизонтально ориентированных углеродных нанотрубок

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Аннотация. В данной работе исследуется влияние геометрических параметров электродов на распределение напряженности электрического поля, необходимого для направленного роста горизонтально ориентированных углеродных нанотрубок методом плазменно-химического осаждения из газовой фазы. Определены оптимальные параметры электродов, обеспечивающие максимальную напряженность электрического поля и высокую эффективность ориентированного роста нанотрубок. Показано, влияние формы электродов (прямоугольных, полукруглых и треугольных) на распределение напряженности поля и ориентацию нанотрубок. Результаты работы способствуют оптимизации процесса роста горизонтально ориентированных углеродных нанотрубок для применения в сенсорах и устройствах нанопьезотроники.

Ключевые слова: углеродные нанотрубки, горизонтальный рост, PECVD, электрическое поле, электрод, моделирование, направленный рост

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Introduction

Carbon nanotubes (CNTs) are among the most promising materials for a wide range of applications due to their exceptional electrical, mechanical, and thermal properties [1−3]. These unique characteristics make CNTs ideal candidates for use in fields such as microelectronics, sensors, energy, and high-strength materials [4−6]. Special attention is given to horizontally aligned carbon nanotubes (HCNTs), which are particularly useful in microelectronic and sensor technologies, as they can be integrated into microelectronic circuits with high controllability and reproducibility [3]. The unique properties of HCNTs make them ideal for applications in energy converters, supercapacitors, flexible electronics, and gas sensors [7−11].

The ability to control the orientation of carbon nanotubes during their growth is critical for their practical applications. Horizontal growth is especially sought after, as it allows CNTs to be integrated into electronic devices and systems with uniform orientation, which significantly impacts their conductivity and other properties, enabling their effective use in high-performance devices [12]. The electric field intensity (EFI), created by electrodes on the substrate, is one of the key factors determining the directionality of CNT growth. The electric field vector influences the orientation of the nanotubes due to their high polarizability along their longitudinal axis [3].

Directed growth of HCNTs involves manipulating the electric field to control the orientation and structure of the nanotubes during their formation. Recent studies have shown that optimizing the geometry of the electrodes can enhance the electric field intensity and, consequently, improve the alignment of the nanotubes. However, achieving stable and high-quality horizontal growth remains a challenging task due to factors such as the electrode shape, their size, and the gap between them.

The aim of this study is to investigate the influence of electrode geometry on the distribution of the electric field that affects the directed growth of horizontally aligned carbon nanotubes using the plasma-enhanced chemical vapor deposition (PECVD) method.

Materials and methods

The study was carried out using numerical modelling in the COMSOL Multiphysics software package, which provides the necessary tools for calculating electric-field distributions. For these purposes, the “Electrostatics” module, intended for analyzing electrostatic fields in specified regions, was used. Modelling was performed for a silicon substrate with various electrode geometries to evaluate their influence on the electric-field distribution in the gap between them.

The modelled structure included a Si substrate measuring 5 × 5 mm and 100 μm thick, coated with a 250 nm SiO_2 layer. The electrodes, made of Mo, were 100 nm thick. The voltage between the electrodes was 1 V. The gap between the electrodes varied from 100 μm to 1 μm, which made it possible to conduct the study for different gap values.

Within the first investigation, the influence of electrode shape on the electric-field distribution in the gap was studied. Three electrode shapes were selected for this purpose: rectangular, semicircular, and triangular. The geometry of the rectangular electrodes was as follows: length 4 mm, width 2 mm. The semicircular electrodes had a base length of 4 mm and a radius of 1.95 mm. The triangular electrodes had a height of 1.95 mm and a base of 3.9 mm, with the apex angle fixed at 90°. The gap between the electrodes was set at 100 μm and remained constant for this experiment. Modelling was carried out with a constant voltage of 1 V applied between the electrodes.

The next stage of the study considered the influence of the geometric parameters of the electrodes on the electric-field distribution. For the semicircular electrodes, the circle radius remained constant at 1.95 mm. Electrode parameters were changed by shifting the lower base by 0.25 mm, which reduced the electrode height from 1.95 mm to 0.45 mm. For the triangular electrodes, the angle (α) opposite the base of the triangle was varied. The angle ranged as follows: α = 15°, 30°, 40°, 60°, 75°, 90°, with corresponding base lengths of 0.5134 mm, 1.045 mm, 1.419 mm, 2.252 mm, 2.458 mm, 3.9 mm. For the rectangular electrodes, length and width were not changed, since theoretical studies showed that altering these parameters would not significantly affect the distribution of electric-field intensity. All changes were made with a constant gap between the electrodes, which was maintained at 100 μm.

The final stage of the study was devoted to analysing the influence of the gap size between the electrodes on the distribution of electric-field intensity. The gap between the electrodes was varied from 1 μm to 100 μm with intermediate values of 10, 25, 50, and 75 μm. The geometric parameters of the electrodes remained unchanged: the rectangular electrodes had a length of 4 mm and a width of 2 mm, the semicircular electrodes had a base length of 4 mm and a radius of 1.95 mm, and the triangular electrodes had a height of 1.95 mm and a base of 3.9 mm with an apex angle of 90°.

Results and discussion

Electric-field distribution versus electrode shape. Fig. 1 illustrates how the geometry of 100-nm-thick Mo electrodes separated by a 100 μm gap governs the magnitude of the electric field (E) in the inter-electrode region. In the rectangular configuration a broad plateau of elevated field is formed; E reaches ≈ 0.0063 V/μm and remains nearly constant across about 60 % of the gap width, a condition favorable for simultaneous nucleation of CNT seeds over large catalyst areas. In the model with triangular electrodes, the electric field magnitude reached $E \approx 0.0055$ V/μm, and the field lines converged toward the sharp electrode vertices. Along the base the magnitude decreases to roughly 85 % of the peak, producing a pronounced guiding component that aligned growing CNTs parallel to the gap axis at the cost of a more localized high-field zone. The semicircular geometry gives the lowest amplitude ($E \approx 0.0046$ V/μm) and a smooth gradient; the absence of corners suppresses field concentration and displaces the high-field zone away from the catalyst surface, which complicates electrostatic control of the growth front.

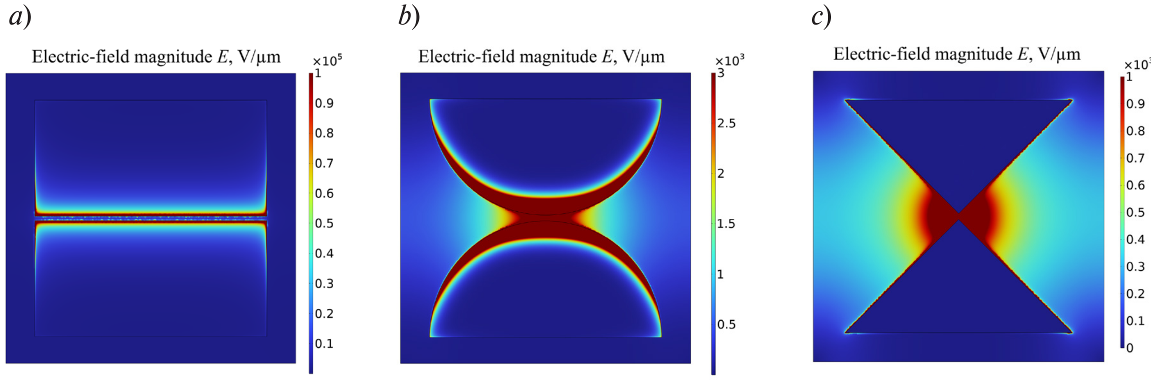

Fig. 1. Surface map of electric-field magnitude E for Mo electrodes with triangular (a), semicircular (b) and rectangular (c) shapes at a gap of 100 μm

Rectangular and triangular electrodes therefore deliver the highest attainable field, whereas semicircular ones are intrinsically limited. The choice between the former two is a trade-off between the area of uniform field (rectangular) and the degree of local enhancement (triangular); this balance must be considered in subsequent optimization of size and gap.

Effect of electrode dimensions. For semicircular electrodes the radius was fixed at 1.95 mm while the height *h* was reduced from 1.95 to 0.45 mm. Lowering *h* increases *E* by only ≈ 6 %; the maximum 0.0046 V/μm occurs at *h* ≈ 1.5 mm, after which the curve saturates. Field lines remain nearly parallel and the high-field area broadens symmetrically, indicating weak sensitivity of the distribution to height at constant radius.

In the triangular case the apex angle *α* (and thus the base length *L*) was varied between 15° (*L* = 0.51 mm) and 90° (*L* = 3.9 mm). At *α* = 90° the field rises to *E* = 0.0055 V/μm. Decreasing the angle to 75° and further to 40° induces an almost linear decline, losing up to 35 % of the maximum at *α* = 40°. Equipotential maps reveal progressive smearing of the field peak along the base, whereas at *α* = 90° the potential gradient is tightly focused near the apex.

a) *b*)

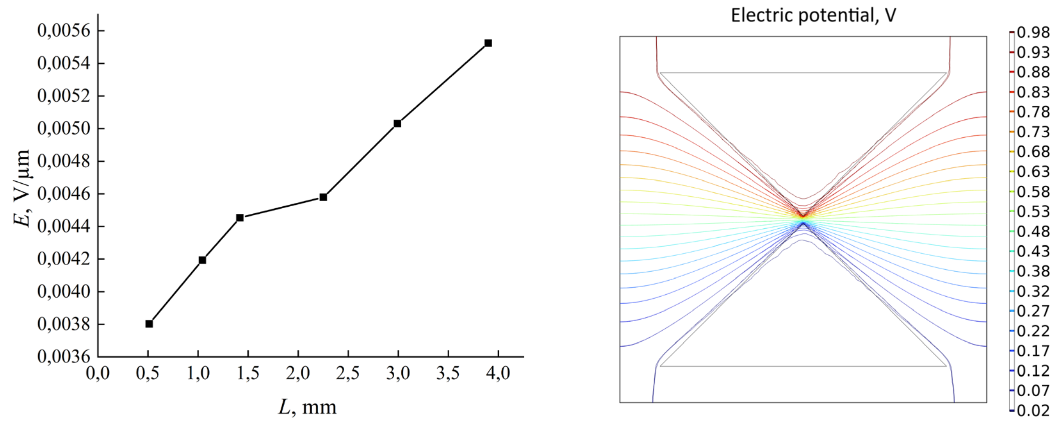

Fig. 2. Dependence of electric-field magnitude *E* on base length *L* for triangular electrodes (*a*); equipotential contours for α = 90° (*b*)

Height variations thus have a secondary effect for semicircular electrodes, whereas the apex angle is the dominant parameter for triangular ones, governing both magnitude and spatial localisation of the field. These trends provide design rules when a high *E* must be combined with a predictable action zone.

Gap-size dependence. Reducing the inter-electrode spacing *d* is the most effective route to elevate *E* in all three geometries. For rectangular electrodes the distribution remains nearly flat: *E* increases from 0.0063 V/μm at *d* = 100 μm to 0.26 V/μm at *d* = 1 μm without pronounced local peaks. Semicircular electrodes respond less linearly: for *d* > 25 μm the rise is moderate, but at *d* ≤ 10 μm stronger gradients emerge; the maximum is limited to 0.12 V/μm and the high-field zone shifts toward the arc, shrinking the useful region.

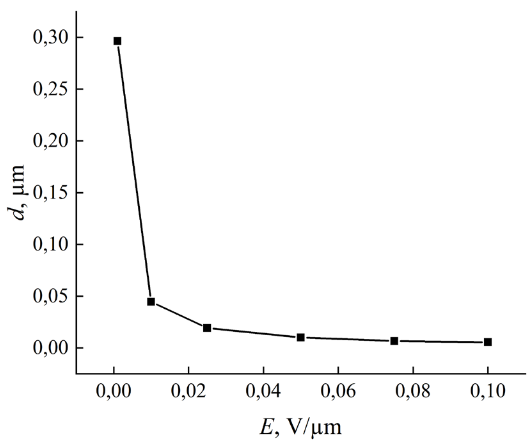

Fig. 3. Dependence of electric-field magnitude *E* on gap *d* for triangular electrodes (α = 90°, *h* = 1.95 mm, *L* = 3.9 mm)

The triangular profile exhibits the steepest dependence. Shrinking *d* from 100 to 1 μm boosts *E* from 0.0055 V/μm to 0.30 V/μm. Simultaneously, the equipotential lines move toward the apex, concentrating the field in a narrow corridor and imposing a strong directional component that aligns CNTs along the gap.

At *d* = 1 μm the triangular design (α = 90°, *h* = 1.95 mm, *L* = 3.9 mm) yields the highest field, 0.30 V/μm, outperforming the rectangular (0.26 V/μm) and semicircular (0.12 V/μm) counterparts.

Local enhancement of the electric field is governed by electrode shape and the presence of sharp vertices that concentrate field lines;

without gap reduction the gains remain modest. Dimensional scaling is critical only for triangular geometry: extending L beyond ≈ 3 mm offers no additional benefit, enabling compact arrays. The gap remains the primary tuning parameter: a tenfold reduction increases E by nearly two orders of magnitude, providing a means to steer horizontal CNT growth at lower anode biases.

The optimal triangular configuration with a lithographically defined 1 μm gap can be integrated on standard-thickness silicon substrates without complicating the process flow. The present findings have been used to design a photomask for an experimental sample featuring the specified triangular electrodes, on which the efficiency of horizontal PECVD growth of carbon nanotubes will be evaluated.

Conclusion

The numerical analysis carried out in COMSOL Multiphysics has provided a comprehensive assessment of how the shape and dimensions of Mo electrodes patterned on a silicon substrate, together with the electrode gap, govern the electric-field distribution that is critical for horizontal PECVD growth of carbon nanotubes (CNTs). Rectangular and, in particular, triangular electrodes generate the highest field strength, while semicircular geometry performs less efficiently because its rounded profile smooths the potential gradient. For triangular electrodes the apex angle is decisive: at $\alpha = 90°$ and a base length of 3.9 mm a strongly localised field enhancement is achieved that can align CNTs along the gap axis. By contrast, varying the height of semicircular electrodes at constant radius has a negligible effect on the field pattern.

The study has shown that the gap width d exerts the greatest influence on the field magnitude. Reducing d from 100 to 1 μm increases the field strength by almost two orders of magnitude; in the optimal triangular configuration the value reaches $E \approx 0.30$ V/μm, sufficient to direct catalyst nanoparticles at reduced anode bias.

The results provide a solid platform for precise control of CNT orientation in micro- and nanoelectronic applications ranging from sensors to interconnects in flexible electronics. Future work will focus on experimental verification of the simulations, exploration of sub-micrometre gaps (d < 1 μm) and optimization of plasma-timing parameters to further enhance the structural integrity and uniformity of CNT arrays.

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