

# Specific Interface Capacitance of Nanocomposite Materials

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**To cite this article:**

Levan Chkhartishvili, Shorena Dekanosidze, Ramaz Esiava, Ia Kalandadze, Dato Nachkebia, Grisha Tabatadze. Specific Interface Capacitance of Nanocomposite Materials. *American Journal of Nano Research and Applications*. Special Issue: Nanotechnologies.

Vol. 5, No. 3-1, 2017, pp. 64-67. doi: 10.11648/j.nano.s.2017050301.24

**Received:** March 29, 2017; **Accepted:** March 30, 2017; **Published:** April 11, 2017

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**Abstract:** Based on a model of interfaces existing between particles of different components, there is obtained the formula to estimate the capacitance of nanocapacitors spontaneously built in nanocomposite materials. The specific (per unit area) interface capacitance depends on the material's characteristics such as: average width of the vacuum gap between the particles of two components, their dielectric constants, absolute values of the space charge average densities in components, and internal voltage corresponding to the difference of work functions of components. The electric capacitance associated with the internal interfaces can significantly affect electronic characteristics and, particularly, dielectric properties of nanocomposite materials.

**Keywords:** Capacitance, Nanocomposite, Interface

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## 1. Introduction

According to the classical electrostatics, decreasing permittivity  $\epsilon$  and thickness  $d$  of a dielectric material, that separates a thin flat capacitor's plates, and increasing their area  $S$  should yield increasing in its capacitance  $C$ :

$$C = \frac{\epsilon_0 \epsilon S}{d} \quad (1)$$

( $\epsilon_0$  is the electric constant). However, for extremely small nanostructures the quantum and the so-called dead-layer effects can change these dependences.

Nano-sized capacitors play an important role in nanoelectronic integrated circuits: they store electrical charge and block direct current while allowing alternating currents to propagate. The nanocapacitor, i.e. capacitor with dimensions of nanoscale, was presented [1] by considering the effects of material properties on its operation: permittivity, dielectric strength, and quantum-electrical phenomena taking place in metal-insulator-metal capacitors on achieving high surface capacitance densities. The concept of nanocapacitor, was discussed [2] in terms of nanostructures some with different from the bulk material properties. Let's describe some examples of constructions proposed so far for nanocapacitors.

The arrays of isolated semispherical nanocapacitors, consisting of porous anodic aluminum oxide layers as dielectric materials and carbon nanotubes as electrodes, were fabricated in [3]. The capacitance calculated using standard semispherical capacitor formula was found to be in agreement with the experimental value. A nanocapacitor with ultra-high capacitance was fabricated [4] using electro-deposited gold nanowires manipulated between two gold microelectrodes by the dielectrophoresis technique. From frequency dependent conductivity, it was seen that the interface exhibits a giant permittivity. The enhancement in permittivity value may be attributed to the formation of a disordered interface containing gold atoms disrupted from the surface of the gold nanowires. The capacitance of a nanocapacitor of dielectric-semiconductor type formed of silicon oxide-silicon layers, deposited alternately with their widths following a Cantor set structure, was calculated numerically [5] and shown that this configuration brings about a nano-hybrid capacitor. Electrostatic capacitors of metal-insulator-metal type fabricated in a cylindrical nanotemplate of anodized anodic aluminum oxide porous film have shown profound increase in capacitance over planar structures. In [6], it was described an electrochemical technique, complementary to the

self-assembled template pore formation process, that provides with significantly reduced local electric field and leakage current densities. The nickel interdigital capacitors were fabricated on top of silicon substrates [7]. The capacitance of such capacitor was optimized by coating the electrodes with a hafnium dioxide nanolayer. The electrical characteristics of solid state nanocapacitors based on a zinc oxide nanowire template were reported in [8]. The fabricated capacitor had a high specific capacitance, an extremely low leakage current density, and good power characteristics.

In some cases, the actual capacitance of nanocapacitors is lower than expected from their geometry. A way to mitigate this negative effect was demonstrated [9] by using graded dielectric films instead of homogeneous films. It was shown that by grading both the permittivity and the elastic constant, one can obtain a palpable enhancement in capacitance.

Recently, it was actually fabricated [10] the thinnest possible nanocapacitor system, essentially consisting of only monolayer materials – h-BN with graphene electrodes – and experimentally demonstrated a significant increase in capacitance below a thickness of ~ 5 nm, more than 100 % of what is predicted by classical electrostatics. Similar example is the liquid exfoliated black phosphorus (BP) nano-flakes taken [11] to make flexible all-solid-state supercapacitors, where the BP-deposited polyethylene terephthalate substrates serve as electrodes. They show excellent specific capacitance and other characteristics even well surpassing their counterparts built on graphene.

As noted, such artificial nanocapacitors are used in nanoelectronics, as well as for storing of electrical energy. The capacitance reduction at small sizes at the first time was theorized [12] as to be originated from the two-dimensional electron gas accumulated at the atomically thin interface (“dead layer”) between insulator and a metallic electrode. The problem how to estimate these capacitances, we have investigated elsewhere [13, 14].

On the other hand, the nanocomposite materials are characterized by very high values of the total specific surface area of interfaces between the particles of different components. Therefore, the electric capacitance associated with the internal interfaces can significantly affect electronic characteristics, and, particularly, dielectric properties of nanocomposite materials. Assessment of the capacity of spontaneously built nanocapacitors, similarly of that for artificial nanocapacitors capacity, is not possible with the standard formula (1). This problem we have already formulated in [15, 16]. Of course, explanation can be simply related to the capacitor thickness: if plates’ linear sizes also are of nanoscale and comparable with  $d$ . For “thick” nanocapacitors, it can be recommended an approach similar to calculations performed by us [17 – 19] to obtain the nanoparticles near-surface field.

In this paper, we intend to solve this problem theoretically, taking into account the impact of two factors: (1) Possibility of formation of the space charge regions on both sides of the interface; and (2) Presence (vacuum) gaps of non-zero thickness between the surfaces of neighboring nanoparticles.

## 2. Model

We choose some part of the approximately flat interface (Figure 1) with area of  $S$  between adjacent particles of two components. Let  $d$  denotes the average width of the vacuum (i.e. with a dielectric constant equal to  $\epsilon = 1$ ) gap between the particles, and by  $D_+$  and  $D_-$  – the thicknesses of positive and negative space charges regions in these components, respectively. Let  $\epsilon_+$  and  $\epsilon_-$  are the dielectric constants, and  $\rho_+$  and  $\rho_-$  – the corresponding absolute values of the space charge average density (for vacuum gap  $\rho = 0$ ).

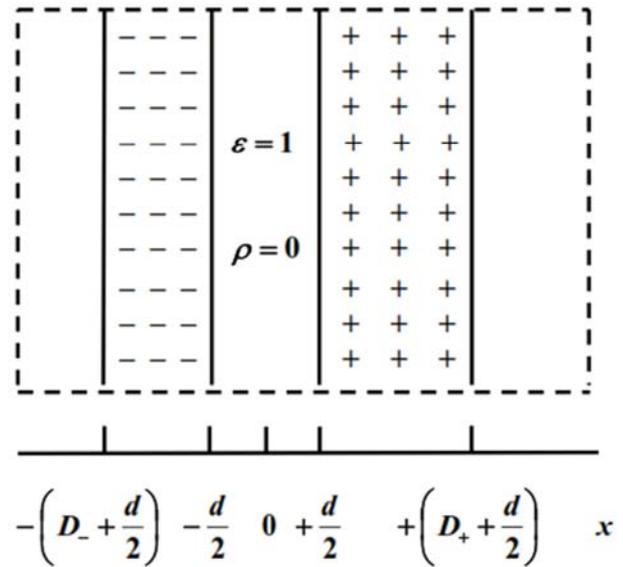


Figure 1. Schematic view of cross section of approximately flat part of interface between particles of different components of nanocomposite material.

Obviously, the parameters  $d$ ,  $\epsilon_+$ ,  $\epsilon_-$ ,  $\rho_+$  and  $\rho_-$  characterize a material, whereas the parameters  $D_+$  and  $D_-$  are also determined by the external voltage drop  $V$  on an interface, if the nanocomposite sample is biased by an external electric field. From the general physical requirement of electrical neutrality,  $\rho_+ D_+ S = \rho_- D_- S$ , it implies the relation between these parameters

$$\rho_+ D_+ = \rho_- D_- \equiv \sigma, \tag{2}$$

where  $\sigma$  is the absolute value of the surface specific charges, on both sides of the interface. Absolute value of the charge  $q$  condensed on a “capacitor plate” equals to

$$q = \sigma S. \tag{3}$$

Electric field strength distribution  $E = E(x)$ , where the axis  $Ox$  is perpendicular to the interface plane, can be calculated from the Gauss theorem:

$$E(x) = \frac{\sigma}{\epsilon_0 \epsilon_-} + \frac{\rho_-}{\epsilon_0 \epsilon_-} \left( \frac{d}{2} + x \right) - \left( D_- + \frac{d}{2} \right) < x < -\frac{d}{2}$$

$$= \frac{\sigma}{\varepsilon_0} - \frac{d}{2} < x < +\frac{d}{2}$$

$$= \frac{\sigma}{\varepsilon_0 \varepsilon_+} + \frac{\rho_+}{\varepsilon_0 \varepsilon_+} \left( \frac{d}{2} - x \right) + \frac{d}{2} < x < + \left( D_+ + \frac{d}{2} \right). \quad (4)$$

### 3. Results and Discussions

If  $V_{\pm}$  is the internal voltage corresponding to the difference in work function of components, the voltages' balance condition

$$\int_{-(D_+ + \frac{d}{2})}^{+(D_+ + \frac{d}{2})} E(x) dx = V_{\pm} + V \quad (5)$$

gives the equation

$$\frac{\sigma(V)}{\varepsilon_0} \left( d + \frac{\sigma(V)}{2} \left( \frac{1}{\varepsilon_+ \rho_+} + \frac{1}{\varepsilon_- \rho_-} \right) \right) = V_{\pm} + V \quad (6)$$

determining absolute value of the surface specific charges in dependence of voltage  $\sigma = \sigma(V)$ . Here it is assumed that  $V \geq -V_{\pm}$  because when  $V < -V_{\pm}$  there are no charges concentrated in the vicinity of the interface:

$$\sigma(V) = 0 \quad V < -V_{\pm}$$

$$= \frac{d}{\frac{1}{\varepsilon_+ \rho_+} + \frac{1}{\varepsilon_- \rho_-}} \left( \sqrt{1 + \frac{2\varepsilon_0(V_{\pm} + V)}{d^2} \left( \frac{1}{\varepsilon_+ \rho_+} + \frac{1}{\varepsilon_- \rho_-} \right)} - 1 \right)$$

$$V \geq -V_{\pm}. \quad (7)$$

Absolute value of the electrical charge condensed on a "capacitor plate" in dependence of voltage  $q = q(V)$  equals to  $q(V) = \sigma(V)S$ . Consequently, we can calculate differential capacitance  $C(V) = dq(V) / dV$  as

$$C(V) = 0 \quad V < -V_{\pm}$$

$$= \frac{\varepsilon_0 S}{\sqrt{d^2 + 2\varepsilon_0(V_{\pm} + V) \left( \frac{1}{\varepsilon_+ \rho_+} + \frac{1}{\varepsilon_- \rho_-} \right)}}$$

$$V \geq -V_{\pm}, \quad (8)$$

Introducing two parameters

$$C_0 = \frac{\varepsilon_0 S}{d} \quad (9)$$

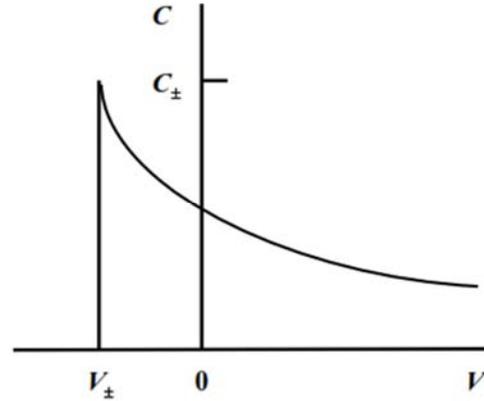
and

$$V_0 = \frac{d^2}{2\varepsilon_0 \left( \frac{1}{\varepsilon_+ \rho_+} + \frac{1}{\varepsilon_- \rho_-} \right)} \quad (10)$$

we can rewrite the expression (8) in the simplified form:

$$C(V) = 0 \quad V < -V_{\pm}$$

$$= \frac{C_0}{\sqrt{1 + \frac{V_{\pm} + V}{V_0}}} \quad V \geq -V_{\pm}, \quad (11)$$



**Figure 2.** Schematic curve of differential capacitance versus voltage for interfaces between particles of different components of nanocomposite material.

The function (11) is shown in Figure 2. One can see that, the differential capacitance at relatively high negative voltages,  $V < -V_{\pm}$ , equals to 0, at  $V = -V_{\pm}$  it reaches its maximum value  $C_0$ , and at sufficiently high positive voltages,  $V \gg V_0$ , vanishes too slowly.

In the limit of low applied voltages,  $|V| \ll V_{\pm}$ , the effective capacitance  $C(0) \equiv C_{\pm}$ , related to the formation of positive and negative space charge regions in neighboring particles of component-materials at the interface between them, equals to

$$C_{\pm} = \frac{\varepsilon_0 \varepsilon_{\pm} S}{d}. \quad (12)$$

It is determined by the effective permittivity  $\varepsilon_{\pm}$  of a gap of "width"  $d$  between these neighboring particles:

$$\frac{1}{\varepsilon_{\pm}} = \sqrt{1 + \left( \frac{1}{\varepsilon_+ \rho_+} + \frac{1}{\varepsilon_- \rho_-} \right) \frac{2\varepsilon_0 V_{\pm}}{d^2}}. \quad (13)$$

Finally, the specific (per unit area) interface capacitance,  $c_{\pm} = C_{\pm} / S$  is found in the following form:

$$c_{\pm} = \frac{\varepsilon_0}{\sqrt{d^2 + 2\varepsilon_0 V_{\pm} \left( \frac{1}{\varepsilon_+ \rho_+} + \frac{1}{\varepsilon_- \rho_-} \right)}} \quad (14)$$

retaining dependences only of the material's characteristics.

## 4. Conclusions

In summary, we have proposed a model for the nanoscale interfaces between particles of different components of a nanocomposite material and based on this model obtained an analytical expression for the capacitance of a nanocapacitor spontaneously built in a nanocomposite material at an interface between adjacent nanoparticles of different components.

The specific capacitance  $c_{\pm}$  of built in nanocapacitors are found to be dependent of average width  $d$  of the vacuum gap between the particles, dielectric constants  $\epsilon_{+}$  and  $\epsilon_{-}$ , absolute values of the space charge average densities  $\rho_{+}$  and  $\rho_{-}$  of these components, and internal voltage  $V_{\pm}$  corresponding to the difference in work function of components.

As the nanocomposite materials are characterized by very high values of the total specific area of interfaces between the particles of different components, the electric capacitance associated with the internal interfaces can significantly affect their electronic characteristics.

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