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Logic gates based on carbon nanotubes

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Abstract. The propagation of a plasmonic pulse signal in carbon nanotubes (CNTs) has been investigated theoretically, and the circuits of plasmonic logic gates "NOT" and "OR" based on CNTs have been proposed. These logic gates represent a complete functional basis for binary logic. The spatial modeling of plasmonic logic gates is performed taking into account the atomic structure of CNTs. The proposed logic gates can be used for plasmonic circuitry in the telecommunication frequency range.

Keywords: nanoplasmonic, logic gate, Mach-Zehnder-type interferometer, carbon nanotube, plasmon interference

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Логические элементы на основе углеродных нанотрубок

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Аннотация. Теоретически исследовано распространение плазмонных импульсных сигналов в углеродных нанотрубках (УНТ) и предложены схемы логических элементов «ИЛИ» и «НЕ» на основе УНТ. Данные логические элементы составляют функциональный базис бинарной логики. Выполнено пространственное моделирование плазмонных логических элементов с учетом атомной структуры УНТ. Предложенные логические элементы могут быть использованы в плазмонных схемах, работающих в телекомуникационном частотном диапазоне.

Ключевые слова: наноплазмоника, логический элемент, интерферометр Маха-Цендера, углеродная нанотрубка, плазмонная интерференция

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Introduction

Plasmonic circuitry currently shows excellent results in increasing the carrier frequencies of pulse signals up to optical ones [1, 2], and increasing clock frequencies in processors up to ten and hundreds of terahertz. But on the other hand, it has relatively large dimensions of plasmonic structures – modulators, logic gates and elements, in particular, based on Mach-Zehnder type interferometers [3–6] with dimensions of tens and hundreds of nanometers. Relatively large sizes of elements are unacceptable in modern circuitry. In addition, metal plasmonic waveguides and elements have large energy losses during heating and due to signal scattering on inhomogeneities. The large size of the elements and losses due to heating hinder the development of plasmonic circuitry.

Carbon nanotubes (CNTs) in which surface waves can be excited have significant advantages over metal plasmonic waveguides: a high level of conductivity and minimal heating losses, and also much smaller transverse dimensions of about 1-2 nm [7-9]. In addition, the wavelength of surface modes in CNTs is an order of magnitude smaller than in plasmonic waveguides when excited by an electromagnetic wave at a telecommunication frequency, which makes it possible to implement gates of plasmonic circuitry based on CNTs with minimal sizes [10].

In this work, the propagation of plasmonic signals in carbon nanotubes is investigated and the schemes of plasmonic logic gates based on nanotubes are proposed. It is possible to create a completely plasmonic logic gate "NOT" representing Mach-Zehnder-type interferometer due to the plasmonic signals follow along the various branches of nanotubes. The plasmonic logic gate "OR" is implemented on the basis of Y-splitter made of CNTs. Such plasmonic structures can be created using well known technologies [8, 9] from CNTs with diameter of 1–2 nm. The proposed logic gates "NOT" and "OR" based on CNTs represent a complete functional basis for binary logic, and can be used for plasmonic circuitry in the telecommunication frequency range. The using of CNTs in the gates of plasmonic circuitry will reduce significantly the size of switching and processing devices operating at telecommunication frequencies.

Nanotube Modes

Expressions for the mode components of a monochromatic ~ $\exp(-i\omega t)$ electromagnetic wave propagating along the CNT can be obtained from the system of Maxwell's equations for a nonmagnetic medium $\mu = 1$ with complex permittivity $\varepsilon = \varepsilon' + i\varepsilon'' = \text{const.}$ Let us represent the permittivity of CNTs according to the Drude model in the form

$$\varepsilon = 1 + \frac{\omega_{e1}^2}{\omega_{01}^2 - \omega^2 - i\gamma_1\omega} - \frac{\omega_{e2}^2}{\omega^2 + i\gamma_2\omega}$$

where $\omega_{e_{1,2}}^2 = 4\pi e^2 N_{1,2}/m$ are the electronic plasma frequencies, ω_{01} is the resonance frequency, $N_{1,2}$ are the concentrations of coupled and free electrons, $\gamma_{1,2}$ are the relaxation frequencies of coupled and free electrons.

For a thin nanotube with radius r_0 when the thickness is much less than the mode wavelength $2r_0 \ll \lambda = 2\pi/\beta$, the solutions of the Maxwell's equations have a physical sense for the field components which tend to zero with increasing distance $r \to \infty$ from the nanotube axis. These solutions are surface evanescent waves (modes).

In the cylindrical coordinate system (r, φ, z) , we have chosen the longitudinal components of the modes outside the nanotube in the form of the MacDonald functions $K_m(wr/r_0)$

$$E_{Z} = A \frac{K_{m}(wr/r_{0})}{K_{m}(w)}, \quad H_{Z} = B \frac{K_{m}(wr/r_{0})}{K_{m}(w)}$$
(1)

then the transverse mode components have the form

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$$E_r = \frac{r_0^2}{w^2} \left[A \frac{-i\beta w}{r_0 K_m(w)} K'_m \left(\frac{wr}{r_0}\right) + B \frac{k_0}{K_m(w)} \frac{m}{r} K_m \left(\frac{wr}{r_0}\right) \right], \qquad (2.1)$$

$$E_{\varphi} = \frac{r_0^2}{w^2} \left[A \frac{\beta}{K_m(w)} \frac{m}{r} K_m\left(\frac{wr}{r_0}\right) + B \frac{ik_0 w}{r_0 K_m(w)} K'_m\left(\frac{wr}{r_0}\right) \right], \qquad (2.2)$$

$$H_{r} = \frac{r_{0}^{2}}{w^{2}} \left[B \frac{-i\beta w}{r_{0}K_{m}(w)} K_{m}' \left(\frac{wr}{r_{0}}\right) - A \frac{k_{0}\varepsilon}{K_{m}(w)} \frac{m}{r} K_{m} \left(\frac{wr}{r_{0}}\right) \right], \qquad (2.3)$$

$$H_{\varphi} = \frac{r_0^2}{w^2} \left[B \frac{\beta}{K_m(w)} \frac{m}{r} K_m\left(\frac{wr}{r_0}\right) - A \frac{ik_0 \varepsilon w}{r_0 K_m(w)} K'_m\left(\frac{wr}{r_0}\right) \right], \qquad (2.4)$$

where the prime denotes the derivative of function with respect to its argument, $m = 0, \pm 1, \pm 2, \dots, w^2 = r_0^2(\beta^2 - k_0^2 \epsilon)$. In order to write the complete expressions for mode components of a thin nanotube, expressions (1) and (2) must be multiplied by $\exp(-i\omega t + im\varphi + i\beta z)$, where β is the propagation constant of the m-th mode.

The dispersion equation for propagation constants β of the nanotube modes can be found using the Leontovich boundary conditions $E_z = \zeta H \varphi$ and $H_z = E_{\varphi}/\zeta$ on the nanotube surface at $\mathbf{r} = r_0$, where $\zeta = \sqrt{(\mu/\epsilon)}$ is the surface impedance (in this case $\mu = 1$). The dispersion equation for the mode propagation constants $\beta_{w}(\omega)$ has the form:

$$K_m^2(w) + \varepsilon \frac{k_0^2 r_0^2}{w^2} K_m'^2(w) = m^2 \frac{r_0^2 \beta^2}{w^4} K_m^2(w)$$
(3)

For modes with azimuthal index m = 0, the dispersion equation (3) takes the form

$$wK_0(w) = \pm i\sqrt{\varepsilon k_0 r_0 K_1(w)}$$
⁽⁴⁾

The mode components in this case look like: *E*-mode

$$E_{r} = i \frac{\beta_{0} r_{0}}{w K_{0}(w)} A K_{1}\left(\frac{wr}{r_{0}}\right), \quad H_{\varphi} = i \frac{\varepsilon k_{0} r_{0}}{w K_{0}(w)} A K_{1}\left(\frac{wr}{r_{0}}\right), \quad E_{z} = A \frac{K_{0}(wr/r_{0})}{K_{0}(w)}, \quad (5)$$

H-mode

$$H_{r} = i \frac{\beta_{0} r_{0}}{w K_{0}(w)} B K_{1}\left(\frac{wr}{r_{0}}\right), \quad E_{\varphi} = -i \frac{k_{0} r_{0}}{w K_{0}(w)} B K_{1}\left(\frac{wr}{r_{0}}\right), \quad H_{Z} = B \frac{K_{0}(wr/r_{0})}{K_{0}(w)}, \quad (6)$$

multiplied by $\exp(-i\omega t + i\beta_0 z)$, where β_0 is the propagation constant of the corresponding mode.

The propagation constant β_0 is determined by the solution of equation (4), where the plus sign must be taken for the *E*-mode, and the minus sign for the *H*-mode. The dependence of the propagation constant β_0 of the *H*-mode on the nanotube radius r_0 with the azimuthal index m = 0 upon excitation at the telecommunication frequency is shown in Fig. 1.



Fig. 1. Dependence of the propagation constant β_0 of the *H*-mode on the nanotube radius r_0 . Dielectric permittivity of CNT $\epsilon = -149.6$ (excluding losses), excitation frequency $\omega = 1.22 \cdot 10^{15} \text{ s}^{-1}$ (wavelength in air $\lambda_0 = 1.545 \text{ }\mu\text{m}$)

The wavelength $\lambda = 2\pi/\beta_0$ of plasmonic *H*-modes varies depending on the nanotube radius r_0 from $\lambda = 32.2$ nm at the diameter of $2r_0 = 1$ nm to $\lambda = 81.1$ nm at the diameter of $2r_0 = 10$ nm. When the nanotube diameter decreases from 10 nm to 1 nm, the ratio of the electromagnetic exciting wavelength to the surface plasmon mode wavelength changes in the range $\lambda_0/\lambda \in (19.48)$. So, the plasmonic carrier wave length is shorter than the exciting electromagnetic signal wavelength about 20–50 times. Near the surface of the nanotube at $r \rightarrow r_0$, the modes with the azimuthal index m = 0 are transformed into plane waves ~ $\exp(-i\omega t + i\beta_0 z)$. In this case, the amplitudes of

the components have the form: for the *E*-mode
$$H_r = -\frac{\beta_0}{\sqrt{\epsilon}k_0}B$$
, $H_r = -\frac{\beta_0}{\sqrt{\epsilon}k_0}B$, $E_z = A$, and for the *H*-mode $H_r = -\frac{\beta_0}{\sqrt{\epsilon}k_0}B$, $E_{\phi} = \frac{1}{\sqrt{\epsilon}}B$, $H_z = B$.

Logic Gates "NOT" and "OR"

The operation principle of the logic gate "NOT" (Fig. 2, a) is based on destructive interference with the simultaneous input of two pulse signals into ports A and B of the logic gate: the clock pulse and a signal corresponding to a logical "unit". The design of the logic gate "NOT" includes two nanoplasmonic interferometers of the Mach-Zehnder type. The principle of operation of the logic gate "OR" (Fig. 2, b) is based on the unhindered passage of pulse signals received at port A or port B of the Y-splitter.



Fig. 2. Plasmonic logic gates based on carbon nanotubes: (*a*) "NOT", (*b*) "OR". A and B are the input ports, Z is the output port, regions I and II show the sections of CNT bending and splitting

The modeling of the spatial configuration of logic gates based on CNTs has been carried out using the HyperChem program. All CNTs in plasmonic logic gates have metallic properties: straight sections of nanotubes with the "armchair" configuration of carbon atoms have chirality indices (6;6), inclined sections have "zigzag" structure (12; 0). The nanotube diameter [9] is

determined in terms of chirality indices (n; m) as $2r_0 = \frac{\sqrt{3}d_0}{\pi}\sqrt{n^2 + m^2 + nm}$, where $d_0 = 0.142$ nm is

the distance between neighboring carbon atoms in graphene plane. So, the diameter of nanotubes in presented logic gates is ≈ 0.81 nm (Fig. 2).

In modeling process the cross-linking of two types of nanotubes "armchair" and "zigzag" has been used for the bending and splitting of the arms of logic gates. This makes it possible to achieve minimal distortion of the hexagonal structure at bending angles of 150 deg and splitting angles of 30 and 60 deg. For coordination in places of the greatest bend, "pentagons" are used for external corners and "heptagons" and "octagons" for internal corners (Fig. 3).

Let us consider in more detail the operation of nanointerferometers in the logic gate "NOT" (Fig. 2, *a*). We assume that the plasmonic pulse at the input to port A or port B of the logic gate has the Gaussian envelope $A(t) = a_0 \exp(-t^2 T_0^{-2}) \exp(-i\omega_0 t)$, where ω_0 is the carrier frequency, T_0 is the pulse duration, $a_0 = \text{const.}$



Fig. 3. Coordination of the CNTs structure in different places: (*a*) 150 deg bending, region I in Fig. 2; (*b*) 60 deg splitting, region II in Fig. 2

At the distance along the axis z = L from the input to the port, each harmonic of the signal acquires the phase delay βL and attenuation αL , where α is the attenuation coefficient, β is the propagation constant. The impulse at length L has the form [11]

$$A(t,L) = \frac{a_0}{2} \frac{\exp(-\alpha L)}{\left(1+\overline{L}^2\right)^{1/4}} \exp\left[-\frac{\left(t-\beta'L\right)^2}{T_0^2\left(1+\overline{L}^2\right)}\right] \cos\left[\omega_0 t - \beta_0 L + \frac{\left(t-\beta'L\right)^2 \overline{L}}{T_0^2\left(1+\overline{L}^2\right)} - \arctan\left(\overline{L}\right)\right]$$
(7)

where $\overline{L} = 2\beta'' L T_0^{-2}$ is the dispersion length.

where A_0

It follows from Eq. (7) that over the length *L* the amplitude of the Gaussian pulse decreases by $\exp(-\alpha L)\left(1+\overline{L}^2\right)^{-1/4}$ times, and the pulse duration increases to $T = T_0\sqrt{1+\overline{L}^2}$.

The pulse phase acquires the temporal modulation $\phi_t = \frac{(t - \beta' L)^2 \overline{L}}{T_0^2 (1 + \overline{L}^2)}$ and the shift $\phi_L = \arctan(\overline{L})$

On the input port B of the logic gate "NOT" (Fig. 2, *a*) a clock pulse is applied at the optical carrier frequency ω . The signal at the input to nanointerferometer B is divided by 50% and propagates further in its arms. With the superposition of two signals, that have passed along the arms of the nanointerferometer B of the same length, the constructive interference takes place, and the logical "unit" appears at the output port Z.

The length of the A nanointerferometer arms is also the same. So, there is the constructive interference of signals at its output port when the signal of logical "unit" is applied to the input port A. The length of the arms of nanointerferometers A and B is different. The superposition of signals that have passed through nanointerferometers A and B leads to the interference of signals at the output port Z, which depends on the phase difference at the outputs of nanointerferometers $A_B = A_A \cos(\omega t - \phi_A) + A_B \cos(\omega t - \phi_B)$.

Let us represent the total signal at the output of the "NOT" gate in the form:

$$A_{AB} = A_0 \cos(\omega t - \phi), \qquad (8)$$
$$= \left[A_A^2 + A_B^2 + 2A_A A_B \cos(\phi_A - \phi_B) \right]^{1/2}, \ \phi = \arctan\left[\frac{A_A \sin(\phi_A) + A_B \sin(\phi_B)}{A_A \cos(\phi_A) + A_B \cos(\phi_B)} \right].$$

A destructive interference of the signal and the clock pulse at the output of the logic gate "NOT" is observed when the phase difference between the signals passed through the nanointerferometers A and B is equal to

$$\phi_A - \phi_B = \beta_0 \left(L_A - L_B \right) + \arctan\left(\overline{L}_A \right) - \arctan\left(\overline{L}_B \right) = \left(2j + 1 \right) \pi, \tag{9}$$

In this case, there is no signal at port Z and the logical "zero" appears at the output port of the gate when the difference in the lengths of the arms of nanointerferometers A and B is equal to $L_A - L_B \approx (2j + 1)\lambda/2$. For the logic gate "NOT", the ratio of the amplitudes of the signal and the clock pulse, as well as the phase shift between them, must ensure that the condition of visibility

of their interference
$$V = \frac{I_{\text{max}} - I_{\text{min}}}{I_{\text{max}} + I_{\text{min}}} \ge \frac{1}{3}$$
, where $I = A_0^2$

Conclusion

A plasmonic signal excited at the telecommunications frequency in CNTs with metallic properties propagates in the form of the surface modes with 6 components (3 electrical and 3 magnetic) described by MacDonald functions. For plasmonic modes with zero azimuthal index, the surface mode splits into the *E*-mode (2 electrical and 1 magnetic components) and the *H*-mode (2 magnetic and 1 electrical component). Near the nanotube surface, plasmon modes transform into the plane waves. The obtained dispersion equation makes it possible to determine the mode propagation constants. The wavelengths of surface plasmon modes depend on the CNT diameter, and the wavelength of the plasmon mode decreases by a factor of ten compared to the wavelength of the exciting electromagnetic wave.

Based on the theoretical analysis of signal propagation in CNTs, the schemes of plasmonic logic gates "NOT" and "OR" are proposed, which represent a complete functional basis for binary logic. The plasmonic logic gate "NOT" consists of two CNT-based Mach-Zehnder-type nanointerferometers, the plasmonic logic gate "OR" is realized on the basis of a CNT Y-splitter.

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