

CHALLENGES and PERSPECTIVES in NANOSCALE ELECTROMAGNETICs

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agnetic waves

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- 1. Introduction
- 2. Nanoelectromagnetics
- 3. Carbon nanotubes: physical properties, conductivity modeling, etc.
- 4. Surface plasmon in CNT
- 5. CNT antenna resonance and THz absorption peak in CNT composites
- 6. Screening effect in Finite-Length MWCNTs
- 7. CNT as THz TWT
- 8. Conclusion & Acknowledgments



What are current trends in electromagnetics?

- Miniaturization of electric circuits components ...
- Energy consumption dropping ...

electronic devices currently account for 15 percent of household

- Opening up the THz & FIR frequency ranges ...
- Advanced EM materials...
- Cross-border and unconventional fields ...

mechanical eigenfrequencies are in GHz and THz range, intracellular heating QD laser







Review Article Nanotechnology for energy-based cancer therapies

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Fig. 1 Very flexible E-textile antenna printed on polymer composite





Prefix "nano-" is the necessary element in all present-day approaches to solve the problems mentioned:

✓ Nanoelectronics,
✓ Nanophotonics,
✓ Nanosensorics,
✓ Nano....
✓ Nano....
✓ Nano....
✓ Nanoelectromagnetics



a research discipline studying the behavior of highfrequency electromagnetic radiation on nanometer scale

Nanoelectromagnetics



is currently emerging as a synthesis of macroscopic electrodynamics and microscopic theory of electronic properties of different nanostructures.



Permittivity of a QD-exciton

After: S.A. Maksimenko, et al., Semicond. Sci. Technol. 15, 491 (2000)

$$\varepsilon_{QD}(\omega) = \varepsilon_{Bulk} + \frac{wg_{QD}}{(\omega - \omega_0 + i / \tau_{dephasing})}$$

$$\begin{split} &w = \pm 1 \quad is \ the \ QD \ population \ (w = 1 \Rightarrow inversion) \\ &g_{QD} \cong 7.10^{14} \, s^{-1} \quad estimated \quad from \ experiment \\ &(g_{QD} \cong 10^{14} \, s^{-1} \ estimated \ from \ laser \ transparancy) \\ &\tau_{depha \sin g} \approx 600 \, ps \quad (Borri) \Rightarrow \end{split}$$



E

$$\mathcal{E}_{QD}(\omega_0) = g_{QD}\tau \approx 4.2 \times 10^5$$

Strong interaction between QD-exciton and EM-field





FUNDAMENTAL CHALENGE in NANOSCALE ELECTROMAGNETICS is

unusual constitutive properties of structural materials due to spatial confinement of the charge carriers motion

or INTERPLAY of SCHROEDINGER and MAXWELL EQUATIONS





Basic Properties of Si, Cu, CNT and GNR

	Si	Cu	SWCNT	MWCNT	Graphene or GNR
Max current density (A/cm²)	-	107	>1x10 ⁹ Radosavijevic, et al., <i>Phys. Rev. B</i> , 2001	>1x10 ⁹ Wei, et al., <i>Appl. Phys. Let.</i> , 2001	>1x10 ⁸ Novoselov, et al., <i>Science</i> , 2001
Melting point (K)	1687	1356	3800 (graphite)		
Tensile strength (GPa)	7	0.22	22.2±2.2	11-63	
Mobility (cm²/V-s)	1400		>10000		>10000
Thermal conductivity (×10 ³ W/m-K)	0.15	0.385	1.75-5.8 Hone, et al., <i>Phys. Rev. B</i> , 1999	3.0 Kim, et al., <i>Phys. Rev. Let.</i> , 2001	3.0-5.0 Balandin, et al., <i>Nano Let.</i> , 2008
Temp. Coefficient of Resistance (10 ⁻³ /K)	-	4	<1.1 Kane, et al., <i>Europhys. Lett.</i> , 1998	-1.37 Kwano et al., <i>Nano Lett.</i> , 2007	-1.47 Shao et al., <i>Appl. Phys. Lett.</i> , 2008
Mean free path (nm) @ room temp.	30	40	>1,000 McEuen, et al., <i>Trans. Nano.</i> , 2002	25,000 Li, et al., <i>Phys. Rev. Let.</i> , 2005	~1,000 Bolotin, et al., Phys. Rev. Let., 2008



Kaustav Banerjee, UCSB



The Handbook of Nanotechnology. Nanometer Structure: Theory, Modeling, and Simulation," Ed. by A. Lakhtakia, SPIE Press, Bellingham, 2004

Chapter 5

Nanoelectromagnetics of Low-dimensional Structures

Sergey A. Maksimenko and Gregory Ya. Slepyan

5.1. Introduction5.2. Electron transport in carbon nanotube

reviews

Nanoelectromagnetics: Circuit and Electromagnetic Properties of Carbon Nanotubes



C. Ruthe

Electron

THE HANDBOOK OF NANOTECHNOLOGY NANDMETER STRUCTURES Theory, Modeling, and Simulation CNT electromagnetics: from Phys Rev to IEEE Trans IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 56, NO. 9, SEPTEMBER 2009 1799 Carbon Nanomaterials for Next-Generation Interconnects and Passives: Physics, Status, and Prospects Hong Li, Student Member, IEEE, Chuan Xu, Student Member, IEEE, Navin Srivastava, Student Member, IEEE, and Kaustav Banerjee, Senior Member, IEEE (Invited Paper) Electromagnetic models 571

Nota Bene!



When we think about CNT as an high-frequency circuit element, we should clearly realize:

- CNT is not a metal even if shows metallic properties;
- Contact barrier determines the total resistivity and has quantum-mechanical nature;
- Finite-length effects are generally of importance in electromagnetic response of single- and multi-walled CNTs

Just an advice: *Do not use standard EM solvers for CNT component modeling without accounting for the peculiar conductivity law (see below)*

55, 273-280 (2001)



Scattering of Electromagnetic Waves by a Semi-Infinite Carbon Nanotube



Gregory Ya. Slepyan, Nikolai A. Krapivin, Sergey A. Maksimenko, Akhlesh Lakhtakia and Oleg M. Yevtushenko

Abstract Scattering of electromagnetic cylindrical waves by an isolated, semi-infinite, open-ended, single-shell, zigzag carbon nanotube (CN) is considered in the optical regime. The CN is modeled as a smooth homogeneous cylindrical surface with impedance boundary conditions known from quantummechanical transport theory. An exact solution of the diffraction problem is obtained by the Wiener-Hopf technique. The differences between the scattering responses of metallic and semiconducting CNs are discussed.

Keywords Carbon nanotube, Diffraction, Impedance boundary conditions, Wiener-Hopf technique At optical frequencies, the cross-sectional radius Rand the length L of actual CNs satisfy the following conditions with respect to the free-space wavenumber k:

$$kR \ll 1$$
, $kL \sim 1$. (1)

Clearly, although the cross-sectional radius is electrically small, the length is electrically large – conditions that are characteristic of wire antennas at microwave frequencies

"Clearly, although the cross-sectional radius is electrically small, the length is electrically large - conditions that are characteristic of wire antennas..." Thus,

an isolated CNT is a wire nano-antenna

The key problem for the CNT electromagnetic response modeling is the conductivity low evaluation





- Dynamical conductivity of an isolated SWCNT
- Polarizability of a finite-length CNT
- Homogenization procedure for CNT composites





Semi classical approximation:

The motion of π -electrons over the CNT surface is described in semiclassical approximation: dispersion law is taken from the quantum-mechanical model, while the motion of the ensemble is described by **the classical kinetic Boltzman equation** for the distribution function : $f(\mathbf{p}, z, t)$

$$\frac{\partial f}{\partial t} + eE_z \frac{\partial f}{\partial p_z} + v_z \frac{\partial f}{\partial z} = J(F(\mathbf{p}); f(\mathbf{p}, z, t))$$

 $v_{z} = \partial \mathcal{E}(\mathbf{p})/\partial p_{z} \qquad \text{is the } \pi\text{-electron velocity}$ $J(F, f) \qquad \text{is the collision integral}$ $F(\mathbf{p}) = \left[1 + \exp\{\mathcal{E}(\mathbf{p})/k_{B}T\}\right]^{-1} \qquad \text{is the Fermi equilibrium}$ distribution functionRelaxation time approximation: $J(F(\mathbf{p}), f(\mathbf{p}, z, t)) \cong \mathcal{V}[F(\mathbf{p}) - f(\mathbf{p}, z, t)]$

 $v = 1/\tau$ is the relaxation frequency. There are different estimates of the relaxation time. In our calculations we take $\tau = 3 \times 10^{-13}$ sec.

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Further we apply standard perturbation procedure of the **Boltzman** equation solution:

Let us set $E_z = \Re[E_z^0 e^{i(hz - \omega t)}]$ in the Boltzmann kinetic equation (1), where h is the axial wavenumber (not to be confused with the Planck constant \hbar) and ω is the angular frequency of the exciting electromagnetic field. Setting f $=F + \Re[\delta f e^{i(hz - \omega t)}]$ with δf as a small quantity to be found, and keeping only linear terms in E_z^0 , we then obtain

$$\delta f = -i \frac{\partial F}{\partial p_z} \frac{e E_z^0}{\omega - h_{V_z} + i\nu}.$$
(4)

The dynamical conductivity law

 $\mathbf{J} = \boldsymbol{\sigma}(\boldsymbol{\omega})\mathbf{E}$

The axial surface current density $J_z = \Re[J_z^0 e^{i(hz - \omega t)}]$ is to be determined by the relation

$$\sigma_{zz}(h,\omega) = \frac{2e^2}{(2\pi\hbar)^2} \iint \frac{\partial F}{\partial p_z} \frac{v_z d^2 \mathbf{p}}{\omega - hv_z + iv} \qquad J_z = \frac{2e}{(2\pi\hbar)^2} \int \int v_z f d^2 \mathbf{p}, \tag{5}$$

with e as the electron charge. Using both foregoing equations, we get

These equations are analogous to constitutive equations of balk conducting media in classical electrodynamics. However, there is significant distinction: In our case we deals with surface current but not with bulk current.

Radial dependence of the conductivity <u>below the optical transitions</u> <u>band</u>



 $R_{\rm cn} = \frac{\sqrt{3}}{2\pi} b \sqrt{m^2 + mn + n^2},$



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The axial conductivity, based on quantum transport theory

$$\sigma_{zz}(\omega) = -\frac{ie^2\omega}{\pi^2\hbar R} \left\{ \frac{1}{\omega(\omega+i\nu)} \sum_{s=1_{1stBZ}}^m \int \frac{\partial E_c}{\partial p_z} \frac{\partial F_c}{\partial p_z} dp_z - 2\sum_{s=1_{1stBZ}}^m \int |R_{cv}|^2 E_c \frac{F_c - F_v}{\hbar^2 \omega(\omega+i\nu) - 4E_c^2} dp_z \right\},$$

Normalized matrix elements of the dipole transition between conduction and valence bands

$$R_{c,\nu}(p_z,s) = -\frac{b\gamma_0^2}{2E_{c,\nu}^2(p_z,s)} \left[1 + \cos(ap_z)\cos\left(\frac{\pi s}{m}\right) - 2\cos^2\left(\frac{\pi s}{m}\right)\right]$$

Electron energy for zigzag CNT (tight-binding approximation):

$$\mathbf{E}_{c,v}(p_z,s) = \pm \gamma_0 \sqrt{1 + 4\cos(ap_z)\cos\left(\frac{\pi s}{m}\right) + 4\cos^2\left(\frac{\pi s}{m}\right)}$$

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overlapping integral γ_0 =2.7 eV, C-C bond length b =1.42 Å



Electrodynamics of carbon nanotubes: Dynamic conductivity, impedance boundary conditions, and surface wave propagation

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4. EM modeling of CNT



Integral equation technique as applied to a finitelength CNT - dipole antenna has been developed in

Conductivity law in the tightbinding approximation, EBCs

a Hallén's-type integral equation

a Leontovich-Levin integral equation

A frequency-domain integral formulation for metallic CNT+conductors PHYSICAL REVIEW B

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Electrodynamics of carbon nanotubes: Dynamic conductivity, impedance boundary conditions, and surface wave propagation

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IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION, VOL. 53, NO. 11, NOVEMBER 2005

Fundamental Transmitting Properties of Carbon Nanotube Antennas

G. W. Hanson, Senior Member, IEEE

PHYSICAL REVIEW B 73, 195416 (2006)

Theory of optical scattering by achiral carbon nanotubes and their potential as optical nanoantennas

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A. Lakhtakia

IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION, VOL. 54, NO. 10, OCTOBER 2006

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An Integral Formulation for the Electrodynamics of Metallic Carbon Nanotubes Based on a Fluid Model



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Electrodynamics of carbon nanotubes: Dynamic conductivity, impedance boundary conditions, and surface wave propagation

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In optical range $\lambda >> b$, $\lambda >> R_{cn}$, b = 0.142 HM

$$\begin{pmatrix} 1 + \frac{l_0}{k^2 (1 + i/\omega\tau)^2} \frac{\partial^2}{\partial z^2} \end{pmatrix} \begin{pmatrix} H_{\phi} |_{\rho=R+0} - H_{\phi} |_{\rho=R-0} \end{pmatrix} = \frac{4\pi}{c} \sigma_{zz} E_z |_{\rho=R}, \\ H_z |_{\rho=R-0} - H_z |_{\rho=R+0} = 0, \ E_{z,\varphi} |_{\rho=R-0} - E_{z,\varphi} |_{\rho=R+0} = 0$$

Spatial dispersion parameter $I_0 \sim 10^{-5}$ for metallic CNTs

Solution of the conductivity problem accounting for the spatial confinement effects couples classical electrodynamics and physics of nanostructures

Surface Waves in CNTs



The problem statement:

consider the propagation of surface waves along an isolated, infinitely long CNT in vacuum. The CNT conductivity is assumed to be axial. The investigated eigenwaves satisfy the Maxwell equations, EBCs and the radiation condition (absence of external field sources at the infinity)

The statement is analogous to the problem of macroscopic spiral slowdown systems for microwave range [L. Weinstein, Electromagnetic waves, 1988].

Dispersion equation of surface waves

$$\frac{\kappa^2}{k^2} K_q(\kappa R) I_q(\kappa R) = \frac{ic}{4\pi R \sigma_{zz}} \left(1 - \frac{\kappa^2 + k^2}{(\omega + i/\tau)^2} c^2 l_0 \right).$$

Surface Wave Propagation



Complex-valued slow-wave coefficient **b** for a polar-symmetric surface wave





What Can We Learn from the Picture?



Carbon Nanotube as an EM device (primarily in the THz range):

- * Electromagnetic slow-wave line: $v_{\rm ph}/c \sim 0.02$
- Dispersionless surface wave nanowaveguide and high-quality interconnects
- Terahertz-range antenna
- Thermal antenna
- Monomolecular traveling wave tube



5. geometrical (antenna) resonances



A vibrator antenna radiates effectively if its length equals to an integer number of halfwaves; for perfectly conducting wire it is $kL = \pi m$, m = 1, 2, 3....

Geometrical resonances: $hL=\pi m$

Because of the large slow-wave effect, $h/k=c/v_{\rm ph}=1/\beta$ ~50, at optical lengths ~ 1 mkm the geometrical resonances are shifted to THz



Experimental observations of THz peak in CNT-based composites





Fig. 1. (a) **EVALUATE:** (b) optical conductivity of oriented nanotubes time along the α_{\parallel} and α_{\perp} directions. The MG fits [Equation (1)] are also presented.

Bommeli F., et al. Synt. Met. **86**, 2307 (1997).



FIG. 3. (Color online) Temperature dependence of the optical conductivity of the two samples.

$$\epsilon(\omega) = \frac{-\omega_p^2}{\omega^2 + i\Gamma\omega} + \sum_i \frac{\omega_{p,i}^2}{(\omega_i^2 - \omega^2) - i\Gamma_i\omega} + \epsilon_{\infty},$$

One can suppose that THz finitelength (antenna) resonances depicted explain THz conductivity peak in CNT composites



(b) Real part of the conductivity together with the Drude and Lorentz contributions to the overall fit (solid line).

T. Kampfrath, phys. stat. sol. (b) 244, No. 11, 3950–3954 (2007)

Homogenization procedure



Consider a dilute composite material comprising CNTs

- randomly dispersed;
- randomly oriented;

- achiral;

Low-frequency approach: Waterman-Truell formula ($kL < \pi/5$)

$$n_{eff}(\omega) = \sqrt{1 + \frac{4\pi f}{3k^2} \sum_{j} F_j(0, \omega, L) N_j(L) dL}$$

$$k = 2\pi / \lambda = \omega / c$$

P. C. Waterman and R. Truell, J. Math. Phys. 2, 512 (1961). A. Lakhtakia, Int. J. Electron. 75, 1243 (1993).

$$F_j(0, \omega, L) = k^2 \alpha_j(\omega, L)$$

polarizability

 $\sigma_{_{eff}}(\omega) = \omega [n_{_{eff}}^2(\omega) - 1]/4i\pi$

is the plane-wave scattering amplitude of an isolated SWCNT at angle θ with respect to the direction of propagation of a plane wave by an SWCNT of type *j* and length L. 29

Comparison with experiment



PHYSICAL REVIEW B 81, 205423 (2010)

Terahertz conductivity peak in composite materials containing carbon nanotubes: Theory and interpretation of experiment

G. Ya. Slepyan, M. V. Shuba, and S. A. Maksimenko C. Thomsen A. Lakhtakia

The predicted amplitudes of resonance lines due to first two optical transitions of the semiconducting SWCNTs coincide reasonably well with the experimental values.

FIG. 3. (Color online) Variations in $\text{Re}(\sigma_{eff})$ with λ at (a) T = 300 K and (b) T = 50 K. Solid lines: experimental data from Fig. 3 of Ref. 18. Dashed lines: theoretical results. When the long-wavelength Approach A was used we set (a) $\nu = 3 \times 10^{13}$ rad s⁻¹ and (b) $\nu = 2.3 \times 10^{13}$ rad s⁻¹.



APPLIED PHYSICS LETTERS 97, 073116 (2010)

Terahertz sensing with carbon nanotube layers coated on silica fibers: Carrier transport versus nanoantenna effects

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V. K. Ksenevich and P. Buka Department of Physics, Belarus State University, Nezalezhnastsi Avenue 4, 220030 Minsk, Belarus D. Seliuta, I. Kasalynas, J. Macutkevic, and G. Valusis Center for Physical Sciences and Technology, A. Gostauto 11, LT 01100 (a)-C. Thomsen distribution (arb. unit) 0 0 0 0 0 A. Lakhtakia 0.0 0.0 2.0 1.01.5 (c) H3 University Park, Pennsylvania 16802-6812 0.0 ŏ.o Length (µm) 0.4 **Dptical density** 0.2 0.0 1000 100

Experimental evidence of localized plasmon resonance in composite materials containing single-wall carbon nanotubes

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Institut für Festkörperphusik, Technische Universität Berlin, Hardenbergs

Nanoengineered Metamaterials Group, Department of Engineering Science and

THz peak: experiment

Direct experimental demonstration of the correlation between the THz peak frequency and the SWCNT length. That, is direct experimental evidence of the slowing down in CNTs and FIR-THz antenna





PHYSICAL REVIEW B 85, 165435 (2012)

<section-header> O. Multiwalled carbon nanotube Description Control of Multiwall carbon nanotubes as waveguides and antennas in the infrarta and the visible regimes M. Y. Shuba, G. Ya. Slepyan, and S. A. Maksimenko Institute for Nuclear Problems, Belarus State University, Bobruiskaya 11, 220050 Minsk, Belarus C. Thomsen A. Lakhtakia Matter Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germania

- 1. the electromagnetic coupling of shells in the MWCNTs;
- 2. the finite length and diameter of MWCNTs.

IEEE Trans. Nanotechnology, 11(3) pp. 554 - 564 (2012)

Transmission Line Model for Multiwall Carbon Nanotubes with Intershell Tunneling

C. Forestiere, A. Maffucci, Senior Member, IEEE, S. A. Maksimenko, G. Miano, G. Ya. Slepyan

metalic shells

Type M:

Multi-walled carbon nanotube



JOURNAL OF APPLIED PHYSICS 108, 114302 (2010)

Radiofrequency field absorption by carbon nanotubes embedded in a conductive host

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Understanding the electromagnetic response of carbon nanotubes (CNTs) in the radio frequency range is very important for experimental development of therapeutic and diagnostic CNT applications, including selective thermolysis of cancer cells and thermoacoustic imaging. In this study, we present the theory of electromagnetic wave scattering by several finite length CNT

O'Connell, *et al.* Cross-section model of an individual fullerene nanotube in a cylindrical SDS micelle, *Science* **297**, 593 (2002)











MWCNT: what new we can expect in electromagnetic response?

- **1. Decrease slowing-down effect**
- 2. Screening effect

Slow-wave coefficient vs the number of shells in MWNT 1: Re(**β**) **CN (9,0)** 10⁴ Гуре А: $\beta = \frac{v_{ph}}{c} = \frac{k}{h} = \frac{k}{h' + ih''}$ 2: $-\text{Re}(\beta)/\text{Im}(\beta)$ emiconducting shells 10² ß **Re** (β) --> 1: 10 **Effect of "graphitization"** 10⁻² 1E-8 1E-7 1E-6 1E-5 1E-4 1E-3 0,01 N -**▲**— Type *M* **(8)** kb Type A 0,06-100 metalic shells (m,0) CNs 0,05 conductivity Гуре M: **Re**(B) 0,1 0,0 0,0 1 0,03 1: Metallic CNs (m=3q) 2: Semiconducting CNs (*m*≠3g) 0,02 1E-3 60 80 100 120 140 0 20 40 m 0,01 12 16 20 Number of shells in MWNT 35

Screening effect in finite-length MWCNT due to strong depolarizing field





Due to the screening effect, the axial surface current reduces in magnitude for successive internal shells.

• The screening effect is stronger for shorter MWNTs

effect • Screening is more pronounced when the electron relaxation time is larger. Indeed, the larger the relaxation time, the larger is the axial surface conductivity and the stronger is the screening effect.

The distribution of the axial surface current along the length of metallic shells of an MWNT exposed to a plane wave with electric field parallel to the CNT axis.

The electric field penetration depth in finite-length MWCNTs



Number N_{ext} is equivalent to the depth of penetration: the larger the value of N_{ext} the more the penetration.



The frequency dependence of the number of external metallic shells providing screening the internal shells

Our calculations demonstrate that in a finite-length MWNT interconnect, the outer metallic shells can be exploited for shielding the remaining inner shells from external spurious radiation, while the inner metallic shells can be used to trnasmit signals.

7. CNT as Nano - TWT









It is well-known, that electron beam in systems which slow down electromagnetic waves can emit radiation (Cherenkov, Smith-Purcell, quasi-Cherenkov mechanisms)

Combination in CNTs of three key properties,

- a strong slowing down of surface electromagnetic waves,
- ballisticity of the electron flow over typical CNT length, and
- extremely high electron current density,

allows proposing them as candidates for the development of nano-sized Chernekov-type emitters







V. Vasnetsov, Knight at the parting of the ways, 1882, State Russian Museum ⁴¹

Problems on the NEM list



- Circuit components and devices design and modeling interconnects, capacitors, inductors, antennae, transmission lines, active components, CNT-QD pairs
- Electromagnetic compatibility on nanoscale non planewave excitations, thermal noise, electromagnetic coupling
- In an an advector of the second se
- Instabilities
 - monomolecular travelling wave tube, active circuit elements
- photothermal effect, medicine

Electromagnetic heating of CNTs and CNT thermo-dynamics, heat transfer on nanoscale

Near-field optics & quantum information processing Parcell effect, lifetime, Few-photon (quantum) circuits, quantum-EM



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ISTC (International Science and Technology Center) B-1708

Thank you for your attention!

