Computational Modeling of Graphene and Carbon Nanotube Structures at Infrared and Optical Regimes

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1. Introduction.

Nowadays, the amount of research time required to develop any emerging technology has decreased from decades to years. This is particularly true for graphene, which has been grown exponentially from almost any reference prior to (Novoselov 2004) to more than 5000 papers and roughly 500 patents in 2011. In this sense, applications in almost any discipline have been envisaged and, when technology has made it possible, manufactured and tested. Those applications have gone beyond the nanotechnology to the macroscopic world, and the usual limits of this exploration are the unavailability of manufacturing processes or the monetary cost of the prototypes. To overcome this situation, it is useful the development of methods able to computationally simulate graphene and carbon nanotubes in macroscopic configurations. Also, the compatibility of this procedures with the actual numerical techniques employed in any discipline will enable the study of nanodimensional properties of the matter from an applied point-of-view.

This chapter attends to the development of a numerical description of the graphene and carbon nanotubes related to electromagnetics. In this sense, it worth to remark that most of the designs including electromagnetic devices based on graphene have been proposed to operate at terahertz, infrared and optical regimes. Then, the numerical description of graphene and carbon nanotubes presented in the first Section is focused in their constitutive parameters at those regimes. The link with the electromagnetic fields is achieved by employing the Maxwell's equations in the second part of the chapter. Taking into account the maturity of the numerical simulators in the field of computational electromagnetics (Sadiku 2010), it is not feasible to explore all possible

approaches in a single chapter. However, the presentation of the algorithms starting for the frequency- or time- domains and the differential- or integral-equation formulations will be helpful to integrate graphene and carbon nanotubes as new electromagnetic materials in the numerical codes, no matter the particular formulation employed by the researchers. As an eventual result, a new generation of electromagnetic devices will be computationally explored, providing thus of a realistic perspective about the possibilities of graphene's technology in the frame of electrodynamics.

2. Theoretical derivation of the conductivity.

As it has been pointed out in the introduction, the main objective of this chapter is to provide a formulation able to translate the nanodimensional electronic transport properties of graphene into the macroscopic Maxwell's equation. To this end, it is considered that the computational electromagnetic modeling of any material of the nature can be achieved by considering the constitutive parameters $(\varepsilon, \mu, \sigma)$. Taking into account the two-dimensional character of graphene and carbon nanotubes, which make the electrical permittivity and magnetic permeability approximately equal to those of the free space, the basis of the proposal is to develop theoretical formulations of the conductivity.

In this sense, several methods have presented in the literature to model graphene (Charlier et al. 2007) (Castro Neto et al. 2009) from a bottom-up perspective, most of them based on the pioneering work (Wallace 1947). Shortly, they employ the quantum mechanics second quantization, supported on the electronic band description, which uses basis functions that

accounts the number of particles occupying each energy state in the complete set of single-particle states. However, the knowledge required to understand this procedures is not usual for engineering people and researchers of other disciplines apart from physics. For this reason, formalism here presented is based on the first quantization, which is more intuitive because is based exclusively on single-particle wave functions. No matter the intermediate formulation, the key step to account for the microscopic electronic transport of carriers into the macroscopic conductivity is the Kubo's equation (Kubo 1956), which enables explicit theoretical equations. Approximations of these equations to simpler forms can be made by assuming different regimes or under certain conditions in the physical parameters (e.g., temperature or chemical potential). Also, the formulation here presented allows to present carbon nanotubes as a particular case of graphene sheers, in which the geometrical periodicity results in a quantization of the transversal momentum.

2.1. Graphene.

Graphene is an allotrope of carbon arranged in a honeycomb structure made out of hexagons whose vertices are occupied by carbon atoms sharing covalent bonds. Electronic properties of graphene can be derived from the band theory of solids. To this end, it is briefly presented a geometrical characterization and a description of energy bands in graphene. Then, a second quantization procedure is applied to achieve the conductivity at any frequency, and finally further approximations for infrared and optical regimes are considered for deriving simpler mathematical expressions of the conductivity.

Geometrically, a hexagonal lattice is a particular case of a rhombic lattice with rectangles which

are $\sqrt{3}$ times as high as wide (Kittel 2004). In this case, a unit-cell contains two non-equivalent atoms (noted as A and B), each one forming a sublattice of identical primitive vectors $\vec{a}_i$:

$$\begin{aligned}\vec{a}_1 &= a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \\ \vec{a}_2 &= a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)\end{aligned} \tag{33.1}$$

where a is the modulus of the lattice vector, which is related to the carbon-carbon distance a_{CC} as $a = \sqrt{3}a_{CC}$. The first Brillouin zone is also hexagonal (Wallace 1947), with reciprocal-lattice vectors $\vec{b}_i$ (Figure 33.1):

$$\begin{aligned}\vec{b}_1 &= \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, 1\right) \\ \vec{b}_2 &= \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, -1\right)\end{aligned} \tag{33.2}$$

[HERE FIGURE 33.1]

In this way, three of the four electrons located in the valence band of any carbon atom are in sp^2 hybridization, i.e., the *2s* orbital is mixed with $2p_x$ and $2p_y$ orbitals to form a total of three σ covalent bonds with neighborhood carbon atoms. The fourth electron, whose $2p_z$ orbital remains independent of the σ bonds, forms a π covalent bond. Conductivity is mainly related to this latter electron, because σ bands are distant of the Fermi level (Figure 33.2), being thus unlikely the transitions from the valence to the conductivity band. For this reason, a carbon atom in graphene has only one electron in valence band.

[HERE FIGURE 33.2]

The energy of the π band can be calculated through the tight binding approximation (Wallace 1947), in which it is assumed that only the interactions between electrons of neighborhood atoms are significant. To this end, it is noted the wave function of the orbital $2p_z$ in an isolated atom as $X(\vec{r})$. Using lattice symmetry, the wave function of any equivalent A-atom can be noted as $X(\vec{r}-\vec{r}_A)$, where $\vec{r}_A$ is the position vector, and similarly for B-atoms as $X(\vec{r}-\vec{r}_B)$. Using the Bloch theorem [1], the periodic Bloch waves for the sublattices A and B are:

$$\begin{aligned}\varphi_1(\vec{r}) &= \frac{1}{\sqrt{N}}\sum_A e^{i\vec{k}\cdot\vec{r}_A} X(\vec{r}-\vec{r}_A) \\ \varphi_2(\vec{r}) &= \frac{1}{\sqrt{N}}\sum_B e^{i\vec{k}\cdot\vec{r}_B} X(\vec{r}-\vec{r}_B)\end{aligned} \tag{33.3}$$

where N is the number of unit-cells of the lattice. Then, the total wave function has the form:

$$\varphi(\vec{r}) = c_1\varphi_1(\vec{r}) + c_2\varphi_2(\vec{r}) \tag{33.4}$$

with c_1 and c_2 constants associated to the normalized wave function φ.

Let H the Hamiltonian of the lattice which allows, among other, the calculus of the energy of an electron in a particular quantum state (Bransden and Joachain, 2000). Taking $\{\varphi_1, \varphi_2\}$ as the basis of the space formed by the lattice wave functions, which satisfies $H\varphi_i = E\varphi_i$ where E is the energy of the electron in the φ_i state, then H can be expressed as:

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \tag{33.5}$$

where $H_{ij} = \int \varphi_i^* H \varphi_j d\vec{r} = H_{ji}^*$.

Also, it is usual in the tight binding approach to neglect the overlapping between orbitals $2p_z$ of different atoms, i.e., $\int X^*\left(\vec{r}-\vec{r}_A\right)X\left(\vec{r}-\vec{r}_B\right)d\vec{r}=0$ for any $A\neq B$. Then, diagonal terms of H are:

$$H_{11}=H_{22}=\frac{1}{N}\sum_{A,A'}e^{-i\vec{k}\cdot\left(\vec{r}_A-\vec{r}_{A'}\right)}\int X^*\left(\vec{r}-\vec{r}_A\right)HX\left(\vec{r}-\vec{r}_{A'}\right)d\vec{r}=\int X^*\left(\vec{r}-\vec{r}_A\right)HX\left(\vec{r}-\vec{r}_{A'}\right)d\vec{r}=\varepsilon_0 \quad (33.6)$$

where geometrical symmetry has been used to state $H_{11}=H_{22}$, and ε_0 corresponds to the energy of an electron on the $2p_z$ in carbon. Regarding the overlap coming from different sublattices, only nearest neighborhoods are considered, which leads to the condition $\int X^*\left(\vec{r}-\vec{r}_A\right)HX\left(\vec{r}-\vec{r}_B\right)d\vec{r}=0$ if A and B are not nearest atoms, and off-diagonal terms of the Hamiltonian are:

$$H_{12}=H_{21}=\frac{1}{N}\sum_{A,B}e^{-i\vec{k}\cdot\left(\vec{r}_A-\vec{r}_B\right)}\int X^*\left(\vec{r}-\vec{r}_A\right)HX\left(\vec{r}-\vec{r}_B\right)d\vec{r}=-t\left(1+e^{i\vec{k}\cdot\vec{a}_1}+e^{i\vec{k}\cdot\vec{a}_2}\right) \quad (33.7)$$

where ε_0, being $\vec{\rho}$ the vector distance between nearest atoms, which does not depend on the particular atom by geometrical symmetry (Figure 33.1).

Taking into account that only energy gaps are needed to characterize the electrical conduction, the ε_0 value can be used as origin of energies. In this way, t is experimentally measured as approximately equal to 2.8 eV, and the Hamiltonian is rewritten as:

$$H=\begin{pmatrix}0 & w\left(\vec{k}\right)\\ w^*\left(\vec{k}\right) & 0\end{pmatrix} \quad (33.8)$$

where $w\left(\vec{k}\right)=-t\left(1+e^{i\vec{k}\cdot\vec{a}_1}+e^{i\vec{k}\cdot\vec{a}_2}\right)$. Eigenvalues and eigenvectors of the matrix are:

$$\varepsilon_{\vec{k},s} = st\sqrt{1+4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right)+4\cos^2\left(\frac{1}{2}k_y a\right)} \tag{33.9}$$

and:

$$\vec{\xi}_{\vec{k},s} = \frac{1}{\sqrt{2}}\begin{pmatrix} -s\dfrac{t}{|t|}e^{i\varphi_{\vec{k}}} \\ 1 \end{pmatrix} \tag{33.10}$$

with $s = \pm 1$, and $\tan\varphi_{\vec{k}} = \dfrac{\mathrm{Im}\left(1+e^{i\vec{k}\cdot\vec{a}_1}+e^{i\vec{k}\cdot\vec{a}_2}\right)}{\mathrm{Re}\left(1+e^{i\vec{k}\cdot\vec{a}_1}+e^{i\vec{k}\cdot\vec{a}_2}\right)}$.

Figure 33.3 shows a three dimensional picture of the dispersion relation arisen from (33.9). The $s=-1$ solution corresponds to the bonding orbitals π, which are filled in the fundamental state, and the $s=1$ solution forms the antibonding orbitals π^* for excited states of the graphene. A similar graph restricted to the $\Gamma-\mathrm{K}$ and $\Gamma-\mathrm{K}$ directions of the first Brillouin zone is presented in Fig. 2, which includes also the σ and σ^* orbitals. At low temperatures only σ and π-bands are occupied, and the Fermi energy is reached at K vertices of the Brillouin zone which also form the Fermi surface for graphene. Furthermore, the choice of $\varepsilon_0 = 0$ as the reference for energies implies that Fermi energy can be considered as zero in the rest of the chapter.

[HERE FIGURE 33.3]

Therefore, the relation dispersion can be carried out considering a small perturbation $\delta\vec{k}$ near the Fermi points of graphene, in the form $\vec{k} = \vec{K} + \delta\vec{k}$. In this way, a series expansion of (33.9) leads to:

$$\varepsilon_{\vec{k},s} = s v_F \hbar \left| \delta \vec{k} \right| \tag{33.11}$$

where the Fermi velocity for graphene is $v_F = \frac{\sqrt{3}a}{2\hbar} t \approx 10^6$ m/s. It worth to remark the linear dependence with $\left| \delta \vec{k} \right|$ in (33.11), illustrated as a zoom in the right part of Figure 33.3, which predicts both ballistic transport and isotropic properties for graphene. Of course, those properties cannot be assumed in general -e.g., in the ultraviolet regime, but they will be certain for the objectives of this chapter.

Regarding the distribution of electrons in the energy bands, the Fermi-Dirac distribution is employed under the assumption that electrons behaves as fermions (Sutton, 1993):

$$f_{\vec{k},s} = \left(1 + e^{\frac{\varepsilon_{\vec{k},s} - \mu_c}{k_B T}} \right)^{-1} \tag{33.12}$$

where k_B is the Boltzmann constant, T is the temperature of the graphene and μ_c is the chemical potential which can be tuned through external fields applied (Fig. 33.4 shows the Fermi-distribution as function of $\vec{k}$ for $\mu_c = 0$).

[HERE FIGURE 33.4]

To derive the conductivity of the graphene, electromagnetic interactions are considered by the total linear momentum $\hbar k + \frac{e}{c} \vec{A}$, where $\vec{A}$ is the electromagnetic potential vector which is related to a harmonic electric field $\vec{E}$ as $\vec{A} = \frac{c}{i\omega} \vec{E}$. Assuming a relatively small electromagnetic momentum, the perturbation method can be applied and mechanical and electromagnetic terms

can be separated in the Hamiltonian as (Zhang et al. 2008):

$$H = H_0 + H' \tag{33.13}$$

where H_0 is given by (33.8), and H' is:

$$H' = \frac{e}{\hbar c}\begin{pmatrix} 0 & -ite^{i\vec{k}\cdot\vec{a}_1} \\ ite^{-i\vec{k}\cdot\vec{a}_1} & 0 \end{pmatrix}\vec{A}\cdot\vec{a}_1 + \frac{e}{\hbar c}\begin{pmatrix} 0 & -ite^{i\vec{k}\cdot\vec{a}_2} \\ ite^{-i\vec{k}\cdot\vec{a}_2} & 0 \end{pmatrix}\vec{A}\vec{a}_2 \tag{33.14}$$

which can be rewritten as:

$$H' = \frac{1}{c}\vec{J}\cdot\vec{A} \tag{33.15}$$

where the components of the current $\vec{J}$ are:

$$J_x = \frac{2ev_F}{\sqrt{\alpha\left(\vec{k}\right)}}\begin{pmatrix} -\sin\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right) & i\left[1+\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right)+\cos\left(k_y a\right)\right] \\ -i\left[1+\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right)+\cos\left(k_y a\right)\right] & \sin\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right) \end{pmatrix} \tag{33.16}$$

and:

$$J_y = \frac{2ev_F}{\sqrt{3\alpha\left(\vec{k}\right)}}\begin{pmatrix} -\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\sin\left(\frac{1}{2}k_y a\right)-\sin\left(k_y a\right) & -i\sin\left(\frac{\sqrt{3}}{2}k_x a\right)\sin\left(\frac{1}{2}k_y a\right) \\ i\sin\left(\frac{\sqrt{3}}{2}k_x a\right)\sin\left(\frac{1}{2}k_y a\right) & \cos\left(\frac{\sqrt{3}}{2}k_x a\right)\sin\left(\frac{1}{2}k_y a\right)+\sin\left(k_y a\right) \end{pmatrix} \tag{33.17}$$

with $\alpha\left(\vec{k}\right) = 1+4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\sin\left(\frac{1}{2}k_y a\right)+4\cos^2\left(\frac{1}{2}k_y a\right)$.

Therefore, Kubo's formulation (Kubo 1956) provides us the components of the conductivity tensor as:

$$\sigma_{\mu\nu} = \sum_{\vec{k}}\frac{1}{\omega}\int dte^{i\omega t}\left\langle J_\mu(t)J_\nu(0) - J_\nu(0)J_\mu(t)\right\rangle \tag{33.18}$$

where $\langle\ \rangle$ means for the trace of the matrix resulting of the product of the corresponding time-

varying density of currents $\vec{J}_x$ and $\vec{J}_y$ and the auxiliary matrix of Fermi-Dirac distribution ρ:

$$\rho = \begin{pmatrix} f_{\vec{k},1} & 0 \\ 0 & f_{\vec{k},-1} \end{pmatrix} \tag{33.19}$$

In our case, (33.18) gives:

$$\begin{gathered} \sigma_{xx} = 4i\frac{e^2 v_F^2}{\pi^2 \omega}\int d\vec{k}\,\frac{\left(1+\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right)+\cos\left(k_y a\right)\right)^2}{\alpha\left(\vec{k}\right)}\, g(\vec{k})\left(f_{\vec{k},1}-f_{\vec{k},-1}\right) \\ \sigma_{yy} = 4i\frac{e^2 v_F^2}{3\pi^2 \omega}\int d\vec{k}\,\frac{\sin^2\left(\frac{\sqrt{3}}{2}k_x a\right)\sin^2\left(\frac{1}{2}k_y a\right)}{\alpha\left(\vec{k}\right)}\, g(\vec{k})\left(f_{\vec{k},1}-f_{\vec{k},-1}\right) \\ \sigma_{xy} = \sigma_{yx} = 0 \end{gathered} \tag{33.20}$$

where $g(\vec{k}) = \left[\frac{1}{\hbar\omega + 2\varepsilon_0\sqrt{\alpha\left(\vec{k}\right)}} - \frac{1}{\hbar\omega - 2\varepsilon_0\sqrt{\alpha\left(\vec{k}\right)}}\right]$, and the approximation $\sum_{\vec{k}} \approx 2\int \frac{d\vec{k}}{(2\pi)^2}$ has been taken.

For low energies, which is the case in terahertz and optical regimes, the occupied states will be located near the Fermi points K. For this reason, the series expansion $\vec{k} = \vec{K} + \delta\vec{k}$ can be repeated leading to approximations $\left(1+\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right)+\cos\left(k_y a\right)\right)^2 \approx \frac{3}{16}k_y^2 a^2$ and $\sin^2\left(\frac{\sqrt{3}}{2}k_x a\right)\sin^2\left(\frac{1}{2}k_y a\right) \approx \frac{9}{16}k_x^2 a^2$, which implies:

$$\sigma = \sigma_{xx} = \sigma_{yy} = i\frac{e^2}{2\pi^2\hbar^2\omega}\int d\vec{k}\left[\frac{1}{\hbar\omega + 2\varepsilon_{\vec{k},1}} - \frac{1}{\hbar\omega - 2\varepsilon_{\vec{k},1}}\right]\left(f_{\vec{k},1}-f_{\vec{k},-1}\right) \tag{33.21}$$

Integral (33.21) can be carried out through change of variables $\varepsilon = \varepsilon_{\vec{k},1} = v_F\hbar\left|\vec{k}\right|$ and

$\theta = \tan^{-1}\left(\frac{k_y}{k_x}\right)$:

$$\sigma = i\frac{e^2}{8\pi^2\hbar^2\omega}\int_0^{2\pi} d\theta \int_0^{\infty} d\varepsilon \left[\frac{1}{\hbar\omega + 2\varepsilon} - \frac{1}{\hbar\omega - 2\varepsilon}\right]\varepsilon\left[f(\varepsilon) - f(-\varepsilon)\right] \tag{33.22}$$

which can be rewritten by integrating by parts and applying that $\varepsilon\left(\frac{\partial f(\varepsilon)}{\partial \varepsilon} - \frac{\partial f(-\varepsilon)}{\partial \varepsilon}\right)$ is an even function as:

$$\sigma = -i\frac{e^2\omega}{\pi}\left[\frac{1}{(\hbar\omega)^2}\int_0^{\infty} d\varepsilon\left(\frac{\partial f(\varepsilon)}{\partial \varepsilon} - \frac{\partial f(-\varepsilon)}{\partial \varepsilon}\right)\varepsilon - \int_0^{\infty} d\varepsilon \frac{f(-\varepsilon) - f(\varepsilon)}{(\hbar\omega)^2 - (2\varepsilon)^2}\right] \tag{33.23}$$

Scattering of electrons can be taking into account by a complex frequency $\omega \to \omega + 2i\Gamma$ (Hanson 2008), where Γ is related to the relaxation time τ for the scattering of electrons in the form $\Gamma = (2\tau)^{-1}$. Then:

$$\sigma = -i\frac{e^2(\omega + 2i\Gamma)}{\pi\hbar^2}\left[\frac{1}{(\omega + 2i\Gamma)^2}\int_0^{\infty} d\varepsilon\left(\frac{\partial f(\varepsilon)}{\partial \varepsilon} - \frac{\partial f(-\varepsilon)}{\partial \varepsilon}\right)\varepsilon - \int_0^{\infty} d\varepsilon \frac{f(-\varepsilon) - f(\varepsilon)}{(\omega + 2i\Gamma)^2 - (2\varepsilon/\hbar)^2}\right] \tag{33.24}$$

which is identical to the lower frequency approximation (including optical and terahertz regime) presented in (Gusynin et al. 2007).

Terms of (33.24) can be identified as a first intraband term, analytically solved as:

$$\sigma = -i\frac{e^2}{\pi\hbar^2(\omega + 2i\Gamma)}\int_0^{\infty} d\varepsilon\left(\frac{\partial f(\varepsilon)}{\partial \varepsilon} - \frac{\partial f(-\varepsilon)}{\partial \varepsilon}\right)\varepsilon = i\frac{e^2 k_B T}{\pi\hbar^2(\omega + 2i\Gamma)}\left[\frac{\mu_c}{k_B T} + 2\ln\left(e^{-\frac{\mu_c}{k_B T}} + 1\right)\right] \tag{33.25}$$

and a interband term, which can be approximated for ($k_B T \ll |\mu_c|, \hbar\omega$), as:

$$\sigma = -i\frac{e^2(\omega + 2i\Gamma)}{\pi\hbar^2}\int_0^{\infty} d\varepsilon \frac{f(-\varepsilon) - f(\varepsilon)}{(\omega + 2i\Gamma)^2 - (2\varepsilon/\hbar)^2} \approx i\frac{e^2}{4\pi\hbar}\ln\left(\frac{2|\mu_c| - (\omega + 2i\Gamma)\hbar}{2|\mu_c| + (\omega + 2i\Gamma)\hbar}\right) \tag{33.26}$$

Equation (33.25) accounts only for intraband response, because $\frac{\partial f(-\varepsilon)}{\partial \varepsilon} = -\frac{\partial f(\varepsilon)}{\partial \varepsilon}$ and thus it can be rewritten as $\sigma = -i\frac{2e^2}{\pi\hbar^2(\omega + 2i\Gamma)}\int_0^\infty d\varepsilon \frac{\partial f(\varepsilon)}{\partial \varepsilon}\varepsilon$ which means that only $s=1$ or $s=-1$ are employed in the calculation, which is not the case for (33.26). Also, it is important to remark for the terahertz regime only (33.24) needs to be considered, and when optical frequencies are considered then both (33.24) and (33.25) should be taken into account.

2.2. Carbon Nanotubes.

Dispersion relation (33.9) remains valid for carbon nanotubes, which can be thought as the enrollment form of graphene. However, then enrollment enforces a geometrical periodicity and the transversal momentum is quantized, simplifying thus the derivation of the conductivity.

Figure 33.5 presents an extended graphene sheet. Any enrolled form is characterized by a vector $\vec{C}_H = m\vec{a}_1 + n\vec{a}_2$ joining to identical carbon atoms which will be located at the same point in the carbon nanotube. Then, $\vec{C}_H$ means for the circumference of the carbon nanotubes, $\left|\vec{C}_H\right| = \sqrt{3}a\sqrt{m^2+mn+n^2}$, and also can be taken as a basis vector in the unit-cell of the carbon nanotubes. Further, translation vector $\vec{T}$ is defined to join the reference point O with the nearest carbon atom, perpendicularly to $\vec{C}_H$. Then, $\vec{T}$ can be expressed as:

$$\vec{T} = t_1\vec{a}_1 + t_2\vec{a}_2 \tag{33.27}$$

where $t_1 = \frac{2m+n}{d_R}$ and $t_2 = \frac{m+2n}{d_R}$, with $d_R = \gcd(2m+n, m+2n)$. In this way, axis of the

carbon nanotube is defined along $\vec{T}$ direction, referenced as z, and the corresponding perpendicular component along $\vec{C}_H$, noted as ϕ.

[HERE FIGURE 33.5]

The wave functions in carbon nanotubes are periodic according to $\vec{C}_H$, and applying Bloch's theorem:

$$\varphi\left(\vec{r}+\vec{C}_H\right)=e^{i\vec{k}\cdot\vec{C}_H}\varphi\left(\vec{r}\right)=\varphi\left(\vec{r}\right) \tag{33.28}$$

which implies:

$$\sqrt{3}\frac{n+m}{2}k_x a+\frac{n-m}{2}k_y a=2\pi s \tag{33.29}$$

For armchair carbon nanotubes ($m=n$), (33.29) is reduced to:

$$\begin{aligned} k_x=k_\phi&=\frac{s}{m}\frac{2\pi}{\sqrt{3}a}\\ k_y&=k_z \end{aligned} \tag{33.30}$$

and for zigzag carbon nanotubes ($m=0$ or equivalently $m=-n$) as:

$$\begin{aligned} k_y=k_\phi&=\frac{s}{m}\frac{2\pi}{a}\\ k_x&=k_z \end{aligned} \tag{33.31}$$

Then, (33.24) still holds for carbon nanotubes, but the transversal momentum quantization has to be taken into account for the integration. To this end we apply the identity $2\pi\int_0^\infty d\varepsilon=\hbar^2\int d\vec{k}v_F^2$, leading to an expression for the intraband conductivity:

$$\sigma_{zz}\left(\omega\right)=-i\frac{4e^2}{\left(2\pi\right)^2\left(\omega+2i\Gamma\right)}\int d\vec{k}\frac{\partial f\left(\varepsilon\right)}{\partial\varepsilon}v_F^2 \tag{33.32}$$

where $\left(\frac{\partial f(\varepsilon)}{\partial \varepsilon}-\frac{\partial f(-\varepsilon)}{\partial \varepsilon}\right)=2\frac{\partial f(\varepsilon)}{\partial \varepsilon}$ has been applied.

[HERE FIGURE 33.6]

For zizag carbon nanotubes (Figure 33.6), (33.31) can be written as $k_\phi=\frac{1}{m}\frac{\pi}{a}s$, and (33.32) is then:

$$\sigma_{zz}(\omega)=-i\frac{8\pi e^2}{(2\pi)^2(\omega+2i\Gamma)ma}\sum_{s=1}^{m}\int dk_z\frac{\partial f(\varepsilon)}{\partial \varepsilon}v_F^2 \tag{33.33}$$

Only Fermi points ($s=m/3$ and $s=2m/3$) have to be considered for the case of metallic zigzag ($m=3n$), and the sum can be reduced to:

$$\sigma_{zz}(\omega)\approx -i\frac{8\pi e^2}{(2\pi)^2(\omega+2i\Gamma)ma}\left(4\int_0^{2\pi/a}dk_z\frac{\partial f(\varepsilon)}{\partial \varepsilon}v_F^2\right)=i\frac{2\sqrt{3}e^2t}{m\pi\hbar^2(\omega+2i\Gamma)} \tag{33.34}$$

Following the same procedure, the conductivity of armchair carbon nanotubes (Figure 33.6) is derived:

$$\sigma_{zz}(\omega)=i\frac{2e^2t}{m\pi\hbar^2(\omega+2i\Gamma)} \tag{33.35}$$

3. Computational models for THz and Optical Regimes.

Once characterized the electronic transport properties of graphene and carbon nanotubes, it remains the question of how to implement these characteristics in computational models of Maxwell's equations. For this purpose, two alternatives may be taken into consideration, a

differential- or a integral-based formulation, and both of them may be formulated in terms of frequency or time-domain approaches. Then, several computational procedures have been developed in the last decades to solve the resulting equations, being the most popular the moment-method solution for integral equations and the finite-difference discretization for differential equations. Other widely extended techniques, such as finite-element or Monte-Carlo algorithms, can be successfully applied and present some computational advantages for particular cases. However, this chapter focuses only with moment-method and finite-difference algorithms because they address most of the common challenging issues to produce stable and accurate results for any computational procedure.

3.1. Differential-equations based formulation.

Any transient electromagnetic wave $\left(\vec{E}(\vec{r},t),\vec{H}(\vec{r},t)\right)$ propagating along a graphene or a carbon nanotube structure accomplishes the Faraday's and Ampère-Maxwell's equations (Taflove 2005), which can be written in the form:

$$\frac{\partial \vec{H}(\vec{r},t)}{\partial t} = -\frac{1}{\mu}\nabla\times\vec{E}(\vec{r},t) - \frac{\sigma^*}{\mu}\vec{H}(\vec{r},t) \tag{33.36}$$

$$\frac{\partial \vec{E}(\vec{r},t)}{\partial t} = -\frac{\sigma}{\varepsilon}\vec{E}(\vec{r},t) + \frac{1}{\varepsilon}\nabla\times\vec{H}(\vec{r},t) \tag{33.37}$$

where the four constitutive parameters $\left(\varepsilon,\mu,\sigma,\sigma^*\right)$ accounts for the specific properties of the any material. In our case, the two-dimensional character of graphene can be considered by a electric permittivity and magnetic permeability equal to free space, a non-lossy magnetic material, and a electric conductivity given by the procedures previously presented -i.e., $\left(\varepsilon_0,\mu_0,\sigma,0\right)$.

However, numerical simulations based on a FDTD procedure for solving equations (33.36) and (33.37) cannot be carried out by a direct substitution of the conductivities (33.25) and (33.26) for graphene, or their quantized form (33.34) or (33.35) for carbon nanotubes, because of the stability issues inherent to the numerical algorithm (Taflove 2005). To avoid these undesired instabilities, an equivalent volume conductivity ε_{eq} is defined, assuming a very small thickness of graphene Δ, in the form $\varepsilon_{eq} = \varepsilon_0 + \frac{\sigma}{j\omega\Delta}$. Of course, the complex relative permittivity values at different frequencies vary under different conditions of (μ_c, Γ, T) (Figure 33.7), but a time-domain formulation of the permittivity is required for any case. A proposed way to achieve this is by formulate a sum of P partial fractions in terms of complex conjugate pole-residue pairs as follows:

$$\varepsilon_{eq} = \varepsilon_0 \varepsilon_\infty + \varepsilon_0 \sum_{p=1}^{P} \left(\frac{c_p}{j\omega - a_p} - \frac{c_p^*}{j\omega - a_p^*} \right) \tag{33.38}$$

where the relative permittivity at infinite frequency ε_∞, the -th pole a_p and residue c_p, are found by employing heuristic techniques (Haupt 2007). Equation (33.38) presents some desirable numerical properties: a) it complies with Kramers-Kronig relationships, which provides it of physical meaning; b) it is unconditionally stable because poles are in the left complex semi-plane; and c) it is versatile for modeling intraband or interband responses, because poles and residuals can describe a Drude or a Lorentz-Drude formulation.

[HERE FIGURE 33.7]

Furthermore, it can be implemented in the time domain by a convolutional or a Auxiliary Differential Equation (ADE) formulation (Han 2006). To this end, the FDTD updating equation for the electric field (the magnetic field-update equation remains unchanged) is:

$$\vec{E}^{n+1} = \vec{E}^{n} + \frac{\Delta t}{\varepsilon_0 \varepsilon_\infty + \sum_{p=1}^{P} \mathrm{Re}\left\{\beta_p\right\}} \left[\nabla \times \vec{H}^{n+1/2} - \sum_{p=1}^{P} \mathrm{Re}\left\{ \left(1 + k_p\right) \vec{J}_p^{\,n} \right\} \right] \tag{33.39}$$

where $\vec{J}_p^{\,n}$ are auxiliary currents introduced by the complex conjugate pole-residue pairs, which are updated by employing:

$$\vec{J}_p^{\,n+1} = k_p \vec{J}_p^{\,n} + \frac{\beta_p}{\Delta t} \left(\vec{E}^{n+1} - \vec{E}^{n} \right) \tag{33.40}$$

and the updating coefficients k_p and β_p depend of the poles and residues as:

$$\begin{aligned} k_p &= \frac{1 + a_p \Delta t / 2}{1 - a_p \Delta t / 2} \\ \beta_p &= \frac{\varepsilon_0 c_p \Delta t}{1 - a_p \Delta t / 2} \end{aligned} \tag{33.41}$$

As an example of results achieved by this method, a terahertz waveguide composed of 50 nm parallel plate distance graphene sheets is simulated in Figure 33.8. At times a steady state, the wavelength can be found from the space-field distribution allows to determine both the wavelength of propagation and the propagation constant for symmetric and anti-symmetric modes.

[HERE FIGURE 33.8]

When carbon nanotubes are considered, the former procedure is no longer adequate because the

small diameter of the enrollment (roughly up to tenths of nanometers) will enforce to excessively fine meshes which would require large supercomputers for practical simulations. To avoid this, it is possible to apply a thin-wire formulation modified to include carbon nanotube structures as it is shown in Figure 33.9. Usual procedure to include thin-wires in FDTD consists in introduce an additional in-cell inductance $\langle L_{incell} \rangle$ and capacitance $\langle C_{incell} \rangle$ per unit length, both related by the transmission-line relationship $\langle C_{incell} \rangle = \varepsilon\mu \langle L_{incell} \rangle$. Considering a carbon nanotube (eventually treated as a thin-wire of radius a and constitutive parameters ε_0, μ_0) placed in a mesh of size $(\Delta x, \Delta y)$, the in-cell inductance is considered as (Berenger 2000):

$$\langle L_{incell,A} \rangle = \frac{\mu_0}{4\pi}\left[\ln\frac{\Delta x^2 + \Delta y^2}{a^2} + \frac{\Delta y}{\Delta x}\arctan\frac{\Delta x}{\Delta y} + \frac{\Delta x}{\Delta y}\arctan\frac{\Delta y}{\Delta x} + \frac{\pi a^2}{\Delta x \Delta y} - 3 \right] \tag{33.42}$$

or (Boutayeb 2006):

$$\langle L_{incell,B} \rangle = \begin{cases} \langle L_{incell,A} \rangle - 0.57\dfrac{\mu_0}{4\pi} & \dfrac{a}{\min(\Delta x, \Delta y)} < 0.3 \\ \langle L_{incell,A} \rangle \dfrac{\Delta x \Delta y}{\Delta x \Delta y - \pi a^2} & \dfrac{a}{\min(\Delta x, \Delta y)} \geq 0.3 \end{cases} \tag{33.43}$$

To account for the conductivity of the carbon nanotube, a circuital circuit model of the conductivity can be employed, in the form:

$$\rho_{CNT} = \frac{1}{\sigma_{CNT}} = R + sL_K + \frac{1}{sC_q} \tag{33.44}$$

where R, L_K, and C_q are, respectively, the resistance, kinetic inductance and quantum capacitance per unit length. In this way, the thin-wire model including CNTs reduces to:

$$\left(\langle L_{incell} \rangle + L_k\right)\frac{\partial I_z}{\partial t} + RI_z + \frac{1}{\langle C_{incell} \rangle + C_q}\frac{\partial Q_z}{\partial z} = \langle E_z \rangle \tag{33.45}$$

which it is ready to be implemented in the FDTD update scheme by discretizing the current I_z and charge Q_z per unit length following the classical procedure given in (Holland 1981).

Results of this method are presented for a dipole of length 20 m and radius 2.712 nm, fed with a Gaussian voltage source at its center at frequencies up to 1 THz. Figure 33.10 plots the time-domain current at the center of the antenna. It can be appreciated the propagation of surface plasmon resonance on the carbon nanotube, with a low frequency resonance mostly related to the kinetic inductance, and a small amplitude of the current due to the large resistance of the ballistic transport of carriers. Also, it becomes apparent that the inductance (33.42) provides results consistent with a formulation based on method-of-moments.

3.2. Integral-equations based formulation.

Maxwell's equations can be rewritten in terms of integral equations, such as the electric field integral equation (EFIE), the magnetic field integral equation (MFIE) or the combined field integral equation (CFIE). All of them can be classified in different ways: attending to the dimensionality of the integrals (volumetric, surface or linear integral equations), in terms of the domain (frequency or time), or depending of the specific unknowns of the equation (current or current-charge integral equations) (Volakis 2012). Usual criteria for the choice among them are related to the nature of the problem. For graphene sheets a surface-based integral equation could be employed, while for carbon nanotubes a linear version could be thought as adequate (and preferable taking into account that required computational resources are related to the dimensionality of the problem). For the domain of solution, frequency-domain solutions are computationally advantageous when single-frequency electromagnetic sources, or at least

narrowband sources, are considered. However, more information for the analysis of physical phenomena is achieved when time-domain is performed, which is more useful for emerging technologies or materials. Regarding the unknowns, the usual choice is the electric current or the density of current, being this a choice more related to the stability and accuracy of the simulations. Finally, specific choice of the integral equations depends of the geometry of the problem, i.e., closed or open geometries. Taking into account that actually manufacturing processes are mature to produce relatively simple graphene sheets or carbon nanotubes, which can be thought as open surfaces, the employment of EFIE is justified.

Therefore, a surface EFIE taking into account the finite conductivity of the graphene can be cast applying appropriate surface impedance boundary conditions (Yuferev 2010). Following the equivalent model for graphene as a volume conductivity ε_{eq}, a graphene layer acts like a thin metal film when $\mathrm{Re}\{\varepsilon_{eq}\}<0$ and electromagnetic waves at any point $\vec{r}$ on the surface of graphene accomplish:

$$\hat{n}\times\vec{E}^{i}(\vec{r})=\hat{n}\times\left(j\omega\mu_0\int_S \vec{J}_s(\vec{r}\,')G(\vec{r},\vec{r}\,')dS'-\frac{1}{j\omega\varepsilon_0}\nabla\int_S \nabla_s'\cdot\vec{J}_s(\vec{r}\,')G(\vec{r},\vec{r}\,')dS'+\frac{\vec{J}_s(\vec{r})}{\sigma(\vec{r})}\right) \quad (33.46)$$

where $\hat{n}$ means for the normal vector to the graphene layer, $G(\vec{r},\vec{r}\,')=\dfrac{e^{-ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}$ is the Green's function connecting source $\vec{r}\,'$ and field $\vec{r}$ points, $\vec{E}^{i}(\vec{r})$ is the incident field which can be external for scattering problems or internal in radiation problems, $\vec{J}_s(\vec{r}\,')$ are the unknown density of currents ($\nabla_s'\cdot$ means for the surface divergence with respect to the primed coordinates), and $\sigma(\vec{r})$ is the conductivity which can be tuned locally by changing the chemical

potential and thus envisaging electromagnetic devices such as surface waveguides (Vakil 2011). Solutions of (33.46) can be achieved by a method-of-moment Galerkin procedure using Rao-Wilton-Glisson basis functions (as long as the graphene remains in planar layers the higher order basis will not increase the accuracy of solutions) (Volakis 2012).

Time-domain counterpart of (33.46) can be derived using inverse Fourier transform:

$$\hat{n}\times\vec{E}^{i}\left(\vec{r},t\right)=\hat{n}\times\left(\frac{\mu_0}{4\pi}\int_S\left[\frac{1}{R}\frac{\partial}{\partial t}\vec{J}_s\left(\vec{r}\,',t-R/c\right)\right]dS'-\frac{1}{4\pi\varepsilon_0}\int_S\left[\frac{1}{R}\int_0^{t-R/c}\left(\nabla_s'\cdot\vec{J}_s\left(\vec{r}\,',\tau\right)\right)d\tau\right]dS'\right)+$$
$$+\hat{n}\times\left(\mathcal{L}^{-1}\left\{\frac{\vec{J}_s\left(\vec{r}\right)}{\sigma\left(\vec{r}\right)}\right\}\right) \tag{33.47}$$

where $R=\left|\vec{r}-\vec{r}\,'\right|$ is the distance between source and field points, c is the velocity of light, $\mathcal{L}^{-1}$ means for the inverse Laplace transform and $t-R/c$ is the retarded time which provides causality to the electromagnetic wave propagation. As it happens with differential formulation, stability issues appears when time-domain solutions are requested. For this reason, the term including conductivity in (33.47) has to be model through as an expansion of Lorentz-Drude series to avoid instabilities. Again, the dispersive equivalent permittivity can be represented as intraband and interband equivalent conductivities (σ^{ib} and σ^{ib}, respectively), from the generic formula:

$$\sigma=\sigma^{ib}+\sigma^{eb}=\frac{f_0\omega_p^2}{s+\Gamma_0}+\sum_{j=1}^{K}\frac{s\varepsilon_0 f_j\omega_p^2}{s^2+s\Gamma_j+\omega_j^2} \tag{33.48}$$

where the intraband (Drude) term contains ω_p corresponding to the plasma frequency associated with the graphene layer. Also, intraband transitions are characterized by an oscillator strength f_0 and a damping constant Γ_0. The term corresponding to the interband contribution obeys a simple

semi-quantum model expressed in a Lorentz form, where K represents the number of oscillators needed to achieve a reasonable fit to the analytical conductivity. Each one of these oscillators is described by three parameters corresponding to their frequency ω_j, strength f_j and damping constant Γ_j. Figure 33.11 presents a comparison of the contributions between typical interband and intraband responses, which shows how the intraband response predominates as getting closer to terahertz regime while optical response is associated only to interband conductivity.

[HERE FIGURE 33.11]

To achieve a numerically efficient procedure, (33.48) can be rewritten in terms of circuital circuit models by defining a set of inductances L_j, capacitances C_j, and resistances R_j, such that

$$\begin{aligned} L_j &= \frac{1}{\varepsilon_0 f_j \omega_p^2} \\ C_j &= \frac{1}{\omega_j^2 L_j} \\ R_j &= \Gamma_j L_j \end{aligned} \tag{33.49}$$

leading to:

$$\sigma = \frac{1}{R_0 + sL_0} + \sum_{j=1}^{K} \frac{1}{R_j + sL_j + \frac{1}{sC_j}} \tag{33.50}$$

Figure 33.12 shows a schematic representation of the circuit model which corresponds to the equivalent conductivity σ of the graphene sheet. Numerical models require one *RL* circuit to represent the Drude term and at least eight *RLC* circuits to represent the Lorentzian responses. It is remarkable that the use of the circuital circuit model to the efficiency of the method does not add a significant computational burden to the solution, as well as provide some physical insight by an inspection of the values corresponding to the specific circuit elements. What is more, it can

be implemented to avoid the employment of any numerical inverse Laplace transform in the code, which may suffer either from inaccuracies, as a result of a numerical truncation of the time-domain response, or from extremely poor computational performance if the complete response of the same term is considered. By using the RLC circuital circuit model (Pantoja et al. 2012), the contribution of each term can be carried out numerically by a trapezoidal integration or a finite difference approximation of the circuital circuit response.

[HERE FIGURE 33.12]

Electromagnetic scattering or radiation problems regarding carbon nanotubes can be solved also by solving a EFIE. Carbon nanotubes usually have a reduced radius/length ratio and, at those frequencies in which the axial current is much larger than the azimuthal one, they can be modeled by the thin-wire approximation. This thin-wire approach can be also simplified for achieving high computational efficiency by considering a particular case of the exact Green's function usually named as the approximate kernel, which takes an advantage of the cylindrical symmetry of the sources and avoids the singularities that arise in the general case, by treating the total current as a filament on the wire axis and enforcing the boundary condition on the wire surface. The use of this approach allows to formulate the modified frequency-domain Pocklington's EFIE in a vacuum (Harrington 1993):

$$\hat{n}\times\vec{E}^{i}(\vec{r}) = \hat{n}\times\left[\frac{1}{\sigma(\vec{r})}\vec{I}(\vec{r}) + \frac{i}{4\pi\varepsilon_0\omega}\int_{C'}\frac{\omega^2}{c^2}\frac{e^{-jkR}}{R}\vec{I}\left(\vec{r}\,'\right)ds' - \frac{i}{4\pi\varepsilon_0\omega}\int_{C'}I\left(\vec{r}\,'\right)\nabla\frac{\partial}{\partial s'}\left(\frac{e^{-jkR}}{R}\right)ds'\right] \quad (33.51)$$

and the corresponding time-domain EFIE is (Miller 1980):

$$\hat{n}\times\vec{E}^{i}(\vec{r},t)=\hat{n}\times\left[\mathcal{L}^{-1}\left\{\frac{1}{\sigma(\vec{r})}\vec{I}(\vec{r})\right\}+\frac{1}{4\pi\varepsilon_0}\int_{C'}\frac{1}{c^2R}\frac{\partial}{\partial t}\vec{I}\left(\vec{r}\,',t'\right)ds'+\frac{1}{4\pi\varepsilon_0}\int_{C'}\frac{\vec{R}}{R^3}\left(\int_0^{t'}\frac{\partial}{\partial r'}I\left(\vec{r}\,',\tau\right)d\tau\right)ds'\right]+$$
$$+\hat{n}\times\left[\frac{1}{4\pi\varepsilon_0}\int_{C'}\frac{\vec{R}}{cR^2}\frac{\partial}{\partial r'}I\left(\vec{r}\,',t'\right)ds'\right] \tag{33.52}$$

where $\vec{I}$ represents the unknown current along the arclength C' of the thin-wire embedded in a vacuum, and $t'=t-\frac{R}{c}$ accounts for the retarded time between the source and field point. It bears remarking that equations (33.51) and (33.52) are no longer valid in the upper part of the visible spectrum, where the axial current no longer dominates because the skin effect begins to become appreciable (Hanson 2006). For this cases, simulations of carbon nanotubes can be made out by employing (33.46) and (33.47).

[HERE FIGURE 33.13]

Results for a carbon nanotube-based dipole, modeled with a RL equivalent circuit corresponding to the Drude model of the intraband conductivity, in the Terahertz regime are presented. Total length *L* of the dipole is 20 μm, with a wire radius of 2.712 nm. Figure 33.13 displays the results for the input impedance over a range of frequencies up to 1 THz. These results demonstrate good agreement between the frequency-domain and time-domain EFIE solutions, and they are consistent with other published results (Hanson 2005). Taking into account the length of the dipole, these results confirm the existence of resonances at lower frequencies in CN dipoles than those corresponding to a standard perfect electric conductor dipole (PEC) of the same length, provided that they could be generated in this range of frequencies. The reason for this fact is found in the slower velocity of the propagation of waves for the carbon nanotubes compared to

the PEC wire. This effect can be analysed by depicting a space-time representation of the currents along the antenna. Figure 33.14 shows the currents along the carbon nanotube dipole as a function of temporal (X axis) and length (Y axis) intervals, where it can be appreciated the formation of lower frequency resonances, mainly due to the inductive propagation of carriers at these frequencies. The electric current reaches the ends of the antenna, forming a traveling wave which returns to the feeding point (at approximately 5000 time intervals), corresponding to the lowest resonant frequency of 0.24 THz shown in Figure 33.14.

[HERE FIGURE 33.14]

4. Conclussions.

This chapter has described numerically the procedures to achieve numerical simulations of graphene and carbon nanotubes in the frame of electrodynamics at terahertz and optical regimes. The method presented is intended to be included in research and commercial software, and for this reason is focused in the formulation of equivalent constitutive parameters. In the first part of the chapter the graphene electronic properties have been achieved by a semi-classical procedure of quantum mechanics, named as first quantization, in which carbon atoms are considered by using quantum wave functions and the electromagnetic field is treated classically. As a result isotropic conductivities for interband and intraband effects are achieved, which covers both the terahertz and optical regime. The second part of the chapter has presented the methodology to account for graphene materials in the most widely employed algorithms in numerical electromagnetics, the finite-difference time-domain and the method-of-moment formulations, as paradigms of the resolution of Maxwell's equation in differential and integral form. Special

attention has been paid to include the complementary time-domain and frequency-domain formulations, because both of them can be useful for simulating complex environments or for analyzing the unusual physical properties of graphene and carbon nanotubes. Results have illustrated both time-domain and frequency-domain responses at terahertz and optical regimes, thus enabling the envisagement of a new generation of electromagnetic devices useful for the nanotechnology.

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Figure labels.

Figure 33.1. Carbon-atoms arrangement in graphene: unit-cell (left) and corresponding first Brillouin zone (right).

Figure 33.2. Energy band structure in graphene.

Figure 33.3. (Left) Energy of electrons in π and π* bands. (Right) Zoom near Fermi points.

Figure 33.4. Fermi-distribution of occupied states for electrons in case of $\mu_c = 0$.

Figure 33.5. Geometrical structure of carbon nanotubes.

Figure 33.6. Quantization of transversal momentum for (left) zigzag and (right) armchair carbon nanotubes.

Figure 33.7. Surface conductivity of graphene for different μ_c. Reprinted with permission from (Lin 2012-2).

Figure 33.8. Electric field of two parallel graphene sheets for symmetric (left) and antisymmetric (right) modes. Reprinted with permission from (Lin 2012-2).

Figure 33.9. FDTD model of a cell including a carbon nanotube. Reprinted with permission from (Lin 2012-1).

Figure 33.10. Current at center of a carbon nanotube dipole of length 20 µm. Reprinted with permission from (Lin 2012-1).

Figure 33.11. Comparison of interband and intraband conductivities at optical regime.

Figure 33.12. A circuital circuit model representing the Lorentz-Drude model.

Figure 33.13. Input impedance of a carbon nanotube dipole of length 20 µm. Reprinted with permission from (Pantoja 2010).

Figure 33.14. Space-time diagram of currents in a carbon nanotube dipole of length 20 µm. Reprinted with permission from (Pantoja 2010).