Response of Semiconductor Nanostructures to a Terahertz Electric Field

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Preface

Since late 1990, the Terahertz technology has become one of the most attractive technologies and gained a very rapid development. Nanostructures based on semiconductors are of considerable current interest due to their novel properties which can be influenced by doping and tailored by geometrical features. Their potential for device and waveguide applications in the terahertz frequency range is well recognized.

This book is a collection of latest research results regarding the response of semiconductor nanostructure to a Terahertz field. The book starts from the review of basic theory of electromagnetic field, the semiconductor physics and the transport theory, which, I believe, could help the readers to better understand the fundamental concepts of our research work. The derivations and analysis for the response of semiconductor object in both static and dynamic field are introduced in most direct way possiblely. Results of computations performed for elementary structures such as nanoplate and nanoparticle are illustrated, which reveal the screening of the internal field while dispersion and absorptions effects are shown by the complex dipole moments. To gain insight into the nature of charge-wave interactions, results based on quasi-static formulation for the electric field are compared with those based on full-wave analysis, with special attention given to the charge and current distributions within the structure. By consideration of the physical process of charge carrier motion and lattice polarization, the equivalent circuit model for semiconductor nanoplate and nanoparticle in the terahertz frequency range are further developed. The equivalent circuit can serve as the basis of analysis for composite structures and aggregates of which the conductive nanoparticle is a constituent. I hope this book could help the reader capture the essences of the response of semiconductor nanostructure to the Terahertz field as well as provide the engineers a more precise and convenience method in analyzing and designing the Terahertz devices and circuits.

In the process of writing this book, I had the fortune of help and support from many people. First, I would like to express my deepest gratitude to my advisor, Dr. Thomas Wong, for his excellent guidance, caring, patience, and providing me with an excellent atmosphere for conducting research. I am most grateful for his teaching and advice, not only for the research work but also for many other things in life. I would not have achieved this far and this book would not have been completed without all the support that I have always received from him. I also would like to express my sincere thanks to Dr. Ming Yan for sharing his valuable experience related to this work with me. Meanwhile, I would like to thank Dr. Hua Wang for his encouragement and kindly help.

It is my pleasure to acknowledge the help of my graduate students, Yongquan Wei, Shuai Ma and Ruiqi Wang, who put great efforts in the preparation work of the manuscript.

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Last but not least, I would like to thank my family members, especially my wife Miao, for their love and encouragement. They give me their unequivocal support throughout the whole period of my graduate study as well as when I started my faculty career, as always, for which my mere expression of thanks likewise does not suffice.

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December 2013

Contents

1 Introduction

Terahertz electromagnetic waves have unique propagation characteristics[1], making them attractive for sensing and subsurface exploration applications[2,3]. Activities in this area is currently enhanced with emerging technology for new signal sources and the rapid progress in the development of synthetic materials with novel waveguiding properties, notably the metamaterials[4~7]. With their high electron density, materials synthesized from metallic particles or aggregates usually exhibit frequency dependence in their electromagnetic properties in the optical region[8,9]. At the same time, arrays of metallic objects suspended in a dielectric medium have been intensely investigated and demonstrated to achieve novel properties in the microwave bands[10]. Because of their lower charge carrier concentrations, semiconductor particles can be expected to have a bulk plasma frequency in the far infrared and terahertz regions, so that they may be utilized to synthesize composite materials whose properties in the terahertz frequency range may be influenced by material composition or the synthesis process[11~14]. To gain insight to the intrinsic nature of interactions of semiconductor nanostructures in the terahertz band, a study of the polarization in a semiconducting nanoplate and a semiconducting nanoparticle subject to the action of an applied electric field in the terahertz range need to be performed.

Elaborate theory for the polarization[16~18] within the elementary structures characterized by different forms of dielectric functions has been developed and successfully applied to account for their scattering properties[19~30]. The dielectric functions employed are often based on that of molecular species containing bound charges that would exhibit orientation or displacement polarizations, leading to a relaxation-type of response function[31] or its derivatives. In the presence of mobile charges as in the case of metallic particles, a complex dielectric function based on the bulk conductivity of the material has been employed to account for the absorption peak observed for metallic particles near their bulk plasma frequencies in the optical region. Indeed, an immediate application of the Mie series solution[32] for the sphere when it was arrived at was in explaining the scattering of light by gold particles. The use of bulk parameters for a material can have its limitation when boundary effects are significant. A typical example is the application of a dielectric function based on bulk conductivity to account for the polarization of a conductive particle in the static limit[33]. To overcome this difficulty, one needs to incorporate the effect of charge accumulation and depletion on the surface of the boundary. This can be accomplished by employing the Boltzmann' s transport formulation[34] to describe the dynamics of the conducting species[35~39], which can be electrons, holes, ions, or other charged entities in the object.

By coupling the field equations to the transport equations of the charge carriers in a conductive particle, screening of the interior electric field by the polarized charges and the dynamics of the charge-field interaction are accounted for. It is often assumed and found to be practical that a quasi-static formulation for the electromagnetic field is adequate for the study of electromagnetic phenomena in particles whose radii are small compare to the free-space wavelength. However, it leads to an unrealistic current distribution when the charge carrier concentration exceeds $10^{20}\,\mathrm{cm}^{-3}$ in a semiconductor particle[40,41]. These difficulties can be overcome by solving for the full-wave solution to the complete set of Maxwell' s equations coupled with the equations of motion for the charge carriers. Therefore, the method of solving the full-wave solution needs to be investigated and determination of applicable range for the quasi-static analysis and the full-wave analysis become a necessity.

Furthermore, as the size of the aggregate increases, a field analysis of composite structures comprising multiple nanoparticles would become rather cumbersome. If, however, an equivalent circuit of a nanoparticle can be arrived at, techniques based on network theory can be applied to aid in the analysis of complex structures, as well as effective medium theory may be employed if the polarizability of an individual particle is attainable by circuit analogy. This enables one to determine the effects of the nanoparticle on its surroundings, which can range from a cluster of similar nanoparticles to waveguiding structures and signal processing components in the terahertz frequency range. The equivalent circuit can also be employed to guide the synthesis of new nanoparticles with heterogeneous internal structures to achieve novel polarisation properties for sensing and terahertz circuitry applications. With this motivation, an investigation of the rationale for the development of the equivalent circuit of a conductive nanoparticle by consideration of the charge carrier transport would appear timely.

In this book, the polarization within a semiconductor nanostructure induced by a terahertz electric field is investigated in terms of a transport model for the motion of the charge carriers, enabling the space charge effects to be revealed. Both analytical and numerical analysis have been conducted. The closed form solutions for the quasi-static formulation and the full-wave formulation have been arrived at and validated by those solutions obtained by the numerical simulation, respectively. The corresponding equivalent circuit model for the conductive particle have been developed to facilitate the analysis for composite structures and aggregates of which the nanoparticle is a constituent. The brief outline of this book is described as follows.

There are seven chapters in this book. The first chapter serves as an introduction, which includes the motivation of this work and the outline of this book.

In chapter 2, a brief review of electromagnetic field theory and the related semiconductor physics is made. The charge transport in semiconductor and the Boltzmann's transport equation which will be used in our analysis are further illustrated.

In chapter 3, the responses of semiconductor nanoplate and nanoparticle in the static electric field are introduced, which are well studied for a long time and could serve as the basis of our research work. The response of elementary semiconductor nanostructures immersed in the quasi-static electric field is investigated in chapter 4. When the object being studied is much smaller than the wavelength, the dynamic fields can be considered as quasi-static. The quasi-static electric field has little retardation over the length scale of interest but is varying with time. Therefore, the Poisson' s equation is still valid in quasi-static analysis. By incorporating the Boltzmann' s transport equation, one can obtain the electric field, charge and current distributions within a semiconductor object immersed in a quasi-static field. In this chapter, the carrier dynamics in the semiconductor objects are briefly reviewed. Analytical solutions of electric field, charge and current distribution inside the conductive nanoplate and nanoparticle are derived by coupling the Poisson' s equation and Boltzmann' s transport equation, respectively. The analytical results are compared with those obtained by numerical method as well.

The quasi-static field analysis is based on the assumption that the object size is much smaller than the wavelength. However, as the doping level is increased, the wavelength inside the semiconductor object will decrease and approach to the size of the object. Under this circumstance, the quasi-static assumption is not appropriate and the wave equation need be utilized to solve for the field distribution instead of the Poisson' s equation. In chapter 5, a full-wave analysis is investigated to give a realistic account of the internal current distribution in a highly conductive nanoparticle. The full-wave formulation encompasses the full set of Maxwell' s equations coupled with the Boltzmann' s equation, along with the boundary conditions for the fields and charges at material interface. An approximate closed form solution for the full-wave formulation is presented, which is fitted to the full-wave numerical simulation results.

In chapter 6, the rationale for the development of the equivalent circuit of a conductive nanostructure by consideration of the charge carrier transport is presented. The total dipole moment obtained from the equivalent circuit is in good agreement with that given by electromagnetic simulation in conjunction with a transport formulation for the carrier motion. All circuit elements are of electrical nature and can be expressed in terms of material parameters. The equivalent circuit can facilitate and dramatically reduce the computation intensity of the analysis for composite structures and aggregates of which the nanostructure is a constituent.

Finally, the summary of this research is made and some suggestions for future work are proposed in chapter 7.

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2 Theoretical Framework

2.1 Electromagnetic Field Theory

The electromagnetic phenomena at macroscopic level are described by Maxwell' s equations, which were published by James C. Maxwell in the nineteenth century. The differential forms of the Maxwell' s equations are:

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} \tag{2.1}$$

$$\nabla \times \boldsymbol{H} = \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t} \tag{2.2}$$

$$\nabla \cdot \boldsymbol{D} = \rho \tag{2.3}$$

$$\nabla \cdot \boldsymbol{B} = 0 \tag{2.4}$$

With the auxiliary relations between electric flux density $\boldsymbol{D}$ and the electric field intensity $\boldsymbol{E}$ *and magnetic flux density* $\boldsymbol{B}$ and magnetic intensity $\boldsymbol{H}$, which are written as:

$$\boldsymbol{D} = \varepsilon \boldsymbol{E} \tag{2.5}$$

$$\boldsymbol{B} = \mu \boldsymbol{H} \tag{2.6}$$

By combining the divergence of the (2.2) and the time derivative of (2.3), the continuity equation can be obtained as:

$$\nabla \cdot \boldsymbol{J} + \frac{\partial \rho}{\partial t} = 0 \tag{2.7}$$

which shows the relation between the charge density and current density.

For a static electric field, since all derivatives with respect to time are vanished Maxwell's equation are reduced to:

$$\nabla \times \boldsymbol{E} = 0 \tag{2.8}$$

$$\nabla \cdot \boldsymbol{D} = \rho \tag{2.9}$$

Under this circumstance, the electric field can be expressed as the gradient of a scalar potential, since its curl is zero everywhere:

$$\boldsymbol{E} = -\nabla\phi \tag{2.10}$$

In most semiconductor materials, the permittivity ε could be treated as a scalar quantity in the absence of strong magnetic field. By substituting (2.10) to (2.3), we can obtain the Poisson's equation as:

$$\nabla^2\phi = -\frac{\rho}{\varepsilon} \tag{2.11}$$

Poisson's equation is used to solve various electrostatic problems. There are many ways to solve the Poisson's equation, where the method of separation of variables is most widely used.

When the electric field is varying with time, the scalar potential alone does not fully account for the electromagnetic field, hence the Poisson's equation becomes inadequate. Instead, by removing the coupling of the Maxwell's equation, one can take the curl of both sides of (2.1):

$$\nabla \times \nabla \times \boldsymbol{E} = \nabla \times \left(-\frac{\partial \boldsymbol{B}}{\partial t}\right) \tag{2.12}$$

The left side can be expanded by a vector identity and right side can be substituted by (2.2):

$$-\nabla^2\boldsymbol{E} + \nabla(\nabla \cdot \boldsymbol{E}) = -\mu\frac{\partial}{\partial t}\left(\varepsilon\frac{\partial \boldsymbol{E}}{\partial t}\right) \tag{2.13}$$

The wave equation can be derived from the above equations as:

$$\nabla^2\boldsymbol{E} - \varepsilon\mu\frac{\partial^2\boldsymbol{E}}{\partial t^2} = \frac{\nabla\rho}{\varepsilon} + \mu\frac{\partial \boldsymbol{J}}{\partial t} \tag{2.14}$$

Equation (2.14) can be also expressed in the time harmonic form as: