ELECTROMAGNETIC ISSUES IN THE MODELING OF ULTRAFAST EXPERIMENTS ON BIASED SEMICONDUCTOR SYSTEMS

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Abstract

Virtually universally computations on the dynamical response of semiconductor devices ignore electrodynamics. However, this cannot be a good approximation if we are to accurately model ultrafast optical experiments in which carriers are photoexcited into a pre-existing electric field. In this paper we explain why this is generally true by considering several example studies, most notably that of Sha et al. [1], and discuss how full-wave electromagnetic models [2] can be used to alleviate these difficulties.

Introduction

All models of semiconductor devices and associated transport issues include some representation of the electromagnetic fields found inside the system. If the spatial and temporal variations in the fields are important, the fields are virtually always computed by using an electrostatic model coupled with an equivalent circuit. Inside the device, a scalar potential is computed by solving Poisson's equation. The rest of the universe is represented by an assumed boundary condition at dielectric interfaces and an equivalent circuit connecting to the device terminals.

The limitations of this electrostatic model are well known. First, the electric scalar potential is an incomplete representation of a time-varying electric field. It should be supplemented with a magnetic vector potential. The electric field will be accompanied by a magnetic field as well. Furthermore, the equivalent circuits used generally ignore various "modes" included in a complete "full-wave" solution to Maxwell's equations.

In this paper we will discuss several experiments which challenge the traditional view that the above limitations are unimportant. We will briefly outline how a full-wave model of such experiments can be developed and used to reinforce the experimentalist's message that electrodynamics directly changes the current flowing through the device.

Ultrafast Optical Experiments on Biased Semiconductors

While there have been many experiments in which femtosecond lasers have been used to probe hot carrier physics, there are comparatively few experiments in which one observed the response of carriers to an applied bias. Yet, this is the situation of greatest interest to the study of electronic devices. It is also this class of experiments that require more than an electrostatic approach in modeling. Please note that the following discussion involves specific examples of nearly universal features of ultrafast optical probes of biased semiconductor systems.

One example of such an experiment is that of Meyer et al. [3] They performed a pump-probe experiment in which the pump pulse excited a photoconductive transient inside a gap found in a micro-strip transmission line deposited on a GaAs epilayer. The probe pulse was used to electro-optically sample the electromagnetic fields propagating down the transmission line. (A related experiment is that of Knox et al. who have a video-tape of experimental data developed by an in-situ probe of the field in their transmission line [4].) Early attempts at modeling such an experiment either used a Monte Carlo transport model in conjunction with a constant electric field [4-6] or supplemented this Monte Carlo model with an equivalent circuit [7].

The most complicated part of this equivalent circuit model is the transmission line model. It is modeled by a frequency-dependent characteristic impedance. The gap model is simpler: a simple constant capacitance. However, the electromagnetically complicated part of the problem is the gap and not the line. There is no simple, frequency dependent capacitance which accurately represents such a gap over the terahertz bandwidth of interest [8]. Indeed, gaps in transmission lines are subjects of ongoing research in computational electromagnetics.

This biased gap is even more complicated than that typically envisioned by the electromagnetics community. While they typically assume that the substrate is a perfect insulator, in these experiments there is a gap substrate current, a photocurrent, that evolves in time. This time-evolving photocurrent in turn is the source for an experimentally observable and potentially useful burst of freely-propagating electromagnetic radiation [9-12]. Obviously, the generation of this freely-propagating radiation cannot be modeled by just a scalar potential. While one could attempt to include it in the form of a radiation resistance, this radiation resistance will not be a simple constant.

Experimentalists design and interpret these experiments at present by using a Hertzian dipole approximation in conjunction with an assumed form for the photocurrent [10]. However, in these experiments the current has a temporal behavior that is affected by the temporal behavior of the field. The initial photocurrent is zero and it rises precisely because the carriers are accelerated by the existing bias field. As this happens, this field will collapse because the power supply is located several feet away, and therefore the only energy flowing into the gap during the subpicosecond acceleration phase is the energy needed to supply the dark current flow through the gap. The electric field collapse and the current growth, are associated with a magnetic field evolution, and Poynting's theorem predicts the experimentally observed burst of electromagnetic radiation. This burst ends when a steady-state in which the current no longer is evolving in time is reached. Therefore the immediate source of energy for the radiation field is not a current source, as assumed in the Hertzian dipole approximation, but rather is the initial bias field of the gap. The question of how the details of the field evolution affect the details of the current evolution is ignored in the Hertzian dipole approach. Lastly, the Hertzian dipole approach ignores the contribution made to the radiation by the electromagnetic discontinuity represented by the gap itself [8].

An excellent example of the importance of these considerations in experiments on biased systems is found in the recent work of Sha et al. They used a pump-probe transient absorption technique to experimentally resolve a ballistic rise in average photocarrier energy [1,13]. They also observed an associated burst of radiation and their data indicates that the energy flowing out of the system through this radiation during the ballistic acceleration phase of their experiment, when few optical phonons are produced, is significant. They present simple arguments that in a purely ballistic acceleration, the conversion of the energy originally stored in the gap field into carrier kinetic energy is expected to occur at a rate comparable to the rate at which the same original energy is radiated into free space [13]. Their experimental data is also consistent with the argument that the experiment is limited at high photocarrier density by the original bias energy of the gap [13].

There is a last important point. The existence of these bursts of freely propagating radiation is not viewed by the experimental community as a headache but rather as an opportunity. Throughout their work you find efforts at utilizing this burst as a probe of either the physics of the generating system or by scattering and transmission measurements as a probe of other systems.

Full-Wave Electromagnetic Models

Over the past several years we have incorporated a full-wave solution to Maxwell's equations in a self-consistent fashion with an ensemble Monte Carlo model of carrier transport

[2,14,15] As the details of the numerical methods have been described elsewhere, here we will discuss several aspects that are important in view of the experimental observation of far-field radiation.

The numerical model which we have selected for use in our studies is the finite-difference time-domain (FD-TD) technique. There are other competing techniques which include spectral domain methods [16] and the method of moments [17] The spectral domain method can be conveniently applied to compute radiation, and propagation in multi-layer geometries. It has some disadvantages however as it models microstrips as infinitesimally thin and perfectly conducting, and assumes that there are no discontinuities in lateral dimensions. The method of moments can be extremely accurate and can be applied to non-planar structures such as waveguides. It has the disadvantage that one must know how to pick certain basis and testing functions, and can have memory size and numerical problems as well. Both the spectral domain method and the method of moments are frequency domain models. The FD-TD model can handle a much wider set of geometries, and operates of course in the time domain. It however is numerically more complicated, does not produce a modal expression of the fields and can be limited by computer memory requirements as discussed below. As the above experiments are characterized by complex, non-uniform geometries, nonlinearity and switching behaviors the FD-TD approach is well suited for studying experiments in ultrafast photoconductivity.

The outgoing radiation field quite naturally appears in the FD-TD approach as it in fact is the most complicated aspect of the electromagnetic boundary conditions. In the finite-difference technique, we eventually must truncate our spatial mesh and the point of concern is that we cannot have a purely artifactual, numerically induced, reflection of the out-going radiation field at this mesh termination. This is avoided by using absorbing electromagnetic boundaries. What these boundaries must in fact absorb is the outgoing radiation field. We have incorporated such boundaries and in fact have developed extensions of them that include the anisotropic dielectric functions associated with an electro-optic sampling crystal. [14]. We found that the choice of boundary condition can have a significant effect on average velocity of a photogenerated carrier inside the gap.

In our approach we must transform the particle model results into continuous charge and current density functions. This is done by simple summations over the particles found in individual mesh cells. An important question is whether or not this is a valid approximation. The main difference between our summation approach and an exact superposition of the fields produced by different sources at that point is the geometrical difference between a set of individual point charges distributed across through the mesh element and an equivalent centrally located charge or current density. The geometrical effect of the distance of the source from the observation point is not included in our simple summation. Provided that the outer reaches of our mesh are sufficiently far from the gap region where the particles are found, that the charge density is not varying significantly on the scale of a mesh element and that we have sufficiently large number of particles found inside a typical mesh element, reasonably accurate results for the outgoing radiation field should be obtained using our approach.

To date, we have made little attempt at vectorizing the electromagnetics code. We also have selected the basic FD-TD techniques by principally concerning ourselves with easy program development. Therefore, we do not feel that our CPU times are particularly meaningful. The key point with regard to computational cost that can be learned from our work is that the arithmetic is dominated by the Monte Carlo particle model while memory usage is dominated by the three-dimensional field solution.

We can however meaningfully compare full-wave electromagnetics with a competing possibility: three dimensional Poisson solvers combined with ensemble Monte Carlo models. In a 3-D Poisson solver one necessarily needs to store charge density and scalar potential. As current density and electric field are parameters of technological importance, they are likely to be stored as well. Therefore, typically 2 scalar and 2 vector quantities are likely to be stored in a 3-D Poisson solution. This is not dramatically different from the 2 scalar and 3 vector quantities which must be stored in a full-wave electromagnetic solution based on field quantities. We therefore expect full-wave solutions to be computationally cost-competitive with 3-D Poisson solvers.

In summary, we have discussed a set of important experiments that cannot be modeled by the typical electrostatic technique. The reasons why this is the case have been discussed in some detail. We have briefly reviewed our existing electrodynamic model for such situations and have discussed how the additional physics required to understand these experiments can be studied using this model. We have further argued that it is an approach which is cost competitive with a 3-D Poisson solver and that it can easily be used with both 2-D and 3-D Monte Carlo models.

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