COMPARISON OF DIFFERENT MODELING APPROACHES FOR GRAPHENE FIELD-EFFECT TRANSISTORS

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Abstract

This work compares two different static approaches to model carrier concentrations in graphene. First, a drift-diffusion based model that approximates 1-D quasi-Fermi levels in the graphene channel (M1). Second, an equilibrium model that expresses carrier concentrations directly as a function of the electric potential (M2). The comparison shows that M1 and a 1-D version of M2 produce the same results at equilibrium. For a non-equilibrium case, deviating results are obtained. The 1-D models assume that carrier concentrations are constant across the thickness of graphene. The work examines the effect of this assumption, by comparing the results of a 1-D and a full 2-D version of M2 at equilibrium. The obtained results are validated against existing literature.

1 Introduction

Graphene-based devices are of great interest in modern research and technology. The successful development and refinement of such devices, like graphene field-effect transistors (GFETs) [1] or high-frequency photodetectors [2], require accurate numerical simulations of their electronic properties. Several models for graphene, based on drift-diffusion equations or hydrodynamic models, have been proposed in recent years [1], [3] and [4].

The focus of this work is to better understand the applicability and relation between the following models: 1) a drift-diffusion based description, that approximates 1-D quasi-Fermi levels in the graphene channel (M1) [1], and 2) a 2-D formulation based on energy levels at equilibrium, where the charge carriers can be directly expressed in terms of the electric potential (M2) [3].

We show numerically that M2 is only valid at equilibrium and that in the nonequilibrium case additional modeling is required, as using quasi-Fermi levels in M1. We further demonstrate the feasibility of an alternative numerical discretization of M1 using the 1-D continuous Galerkin method, combined with a successive under-relaxation technique, to solve the resulting nonlinear system of equations.

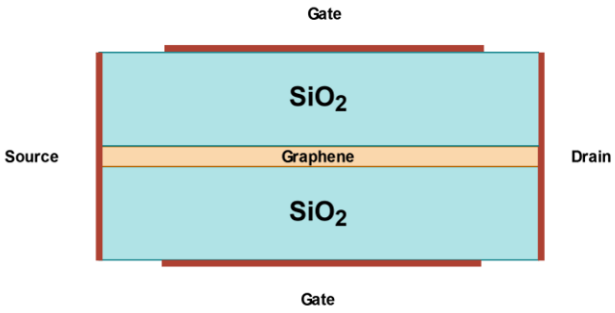

Figure 1: Artist's view of the studied GFET structure.

2 Numerical Modeling

We consider the well-understood GFET structure depicted in Figure 1, first introduced in Reference [1]. The structure consists of a graphene sheet between two oxide layers. Four copper contacts are attached to the structure, to influence the carrier concentrations in the graphene channel and consequently its electric conductivity.

To simulate the structure, a 2-D Poisson equation for the electric potential in the complete domain is coupled with a model for the carriers in the graphene channel only [1], [3].

In Reference [1], the authors propose to model the carrier concentrations in graphene using static bipolar 1-D continuity equations along the center of the channel. Electric currents are expressed in terms of gradients of 1-D quasi-Fermi levels, and the dispersion relation in graphene near the Dirac-point is used to analytically estimate the carrier concentrations based on the quasi-Fermi levels and electric potential. The 1-D carrier concentrations are extended to the 2-D domain by assuming that carrier concentrations are constant throughout the thickness of the graphene region.

In Reference [3], the authors propose an alternative static model for the carrier concentrations. Using the dispersion relation in graphene, the carrier concentrations are directly estimated as a function of the electric potential in the full 2-D graphene domain, resulting in concentrations that vary throughout the thickness.

We implemented a continuous Galerkin 2-D finite element (FE) discretization of the Poisson equation coupled with either a 1-D FE discretization of the

continuity equations in M1 or the analytic formula of M2. The strong nonlinearity in both models is handled using a successive under-relaxation scheme.

We used the size and material parameters of the GFET structure as proposed in Reference [1]. The comparison has been carried out in two steps. First, we compared M1 with a 1-D version of M2, assuming constant carrier concentration across the thickness of graphene. Second, we examined the effect of this assumption on the results of M2.

3 Results

Figure 2 shows the estimated electric potential along the center of the graphene channel, computed by the two models for the analyzed GFET structure, with a gate voltage of 1.5V, source voltage of 0V and a drain voltage (V_D) of 0V or 0.2V, respectively.

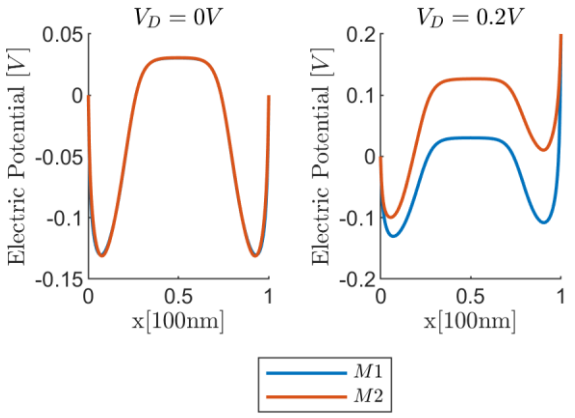

Figure 2: Electric potential along the center of the graphene channel computed by M1 and M2 for V_D=0V (left) and V_D=0.2V (right).

As opposed to the equilibrium case (V_D=0V), where the computed potentials match very well, considerable differences arise in the non-equilibrium case (V_D=0.2V). A similar behavior is also obtained for the simulated carrier concentrations. The computed concentrations for M1 are in good agreement with the results reported in Reference [4], highlighting the validity of the alternative discretization approach and treatment of the nonlinearity.

This comparison shows that M2 can be used to produce fast and accurate results for equilibrium configurations, but additional modeling efforts, as in M1 using quasi-Fermi levels, seem necessary for accurate device characterization out of equilibrium. Indeed, a direct link between the carrier concentrations and the electric potential can generally only be assumed at equilibrium with a constant Fermi level in the structure [5].

We further examined the effect of the assumption that the carrier concentrations are constant across the thickness of the graphene channel. Figure 3 shows the electron densities along the center of the channel computed by M2 for the equilibrium case (V_D=0V), depending on whether we use the above assumption or the full 2-D carrier model, corresponding to a constant Fermi level in the complete channel domain. The 1-D version produces larger carrier concentrations along the center of the channel.

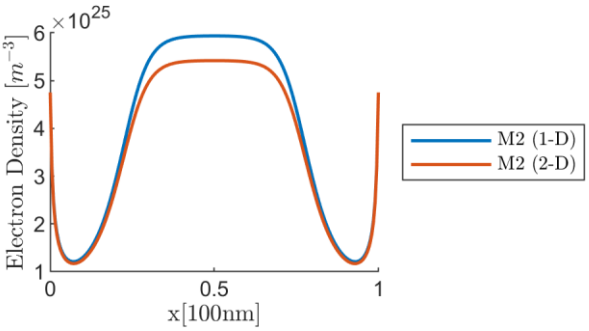

Figure 3: Electron concentration along the center of the graphene channel computed by the 1-D and 2-D version of M2 for V_D=0V.

4 Conclusion and Outlook

We compared results of a Drift-Diffusion-based model (M1) and a simple equilibrium model (M2), highlighting the effect of modeling quasi-Fermi levels for out of equilibrium configurations. We further demonstrated for an equilibrium configuration, that the assumption of uniform carrier concentrations across the graphene thickness yields results deviating from a full 2-D equilibrium description.

At the conference, we aim to present additional results for a full 2-D quasi-Fermi level-based model of graphene. We believe that such a model is particularly important to better understand the effects of edge- and top-contacts, previously suggested in many graphene-based devices.

References

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