Computer Physics Communications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Simulating electron wave dynamics in graphene superlattices exploiting parallel processing advantages☆

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ARTICLE INFO

Article history:
Received 31 January 2017
Received in revised form 8 June 2017
Accepted 24 August 2017
Available online xxxx

Keywords:
Graphene Superlattice (GSL)
Electron wave dynamics
Finite-Difference Time-Domain (FDTD)
Open Computing Language (OpenCL)
Graphics Processing Unit (GPU)
Parallel Processing
Multi-GPU

ABSTRACT

This work introduces a parallel computing framework to characterize the propagation of electron waves in graphene-based nanostructures. The electron wave dynamics is modeled using both "microscopic" and effective medium formalisms and the numerical solution of the two-dimensional massless Dirac equation is determined using a Finite-Difference Time-Domain scheme. The propagation of electron waves in graphene superlattices with localized scattering centers is studied, and the role of the symmetry of the microscopic potential in the electron velocity is discussed. The computational methodologies target the parallel capabilities of heterogeneous multi-core CPU and multi-GPU environments and are built with the OpenCL parallel programming framework which provides a portable, vendor agnostic and high throughput-performance solution. The proposed heterogeneous multi-GPU implementation achieves speedup ratios up to 75x when compared to multi-thread and multi-core CPU execution, reducing simulation times from several hours to a couple of minutes.

Program summary

Program title: GslSim.
Program Files doi: http://dx.doi.org/10.17632/prmfv63nj6.1
Licensing provisions: GPLv3.
Programming language: C, OpenCL and Matlab for results analysis.
Nature of problem: Computing the time evolution of electron waves in graphene superlattices is a time consuming process due to the high number of necessary nodes to discretize the spatial and time domains.
Solution method: We develop a simulator based on the C/OpenCL standards to study the time evolution of electron waves in graphene superlattices by exploiting hardware architectures such as graphics processing units (GPUs) to speedup the computation of the pseudospinor.

1. Introduction

Graphene is a carbon-based two-dimensional material where the carbon atoms are arranged in a hexagonal lattice. Recent studies suggested the possibility of controlling the electronic properties of graphene by applying an external periodic electrostatic potential on its surface with a patterned metallic gate, among other possibilities. These nanostructured materials are known as graphene superlattices (GSLs) [1–10]. The low-energy dynamics of the electrons in GSLs is typically characterized by the massless Dirac equation [11–13] whose solution is usually numerically determined, for instance with the Finite-Difference Time-Domain (FDTD) method [14,15]. The FDTD algorithm is used in a variety of scientific domains and the associated computational complexity is determined by the nature of the problem. Previous works in the context of electromagnetism have shown that it is possible to obtain impressive speedup ratios (on the order of 20–100x) with a single graphics processing unit (GPU) implementation, e.g., [16,17]. Furthermore, a multi-GPU environment enables additional speedup gains, e.g., [18,19].

The application of the FDTD scheme to the electron wave propagation in graphene platforms typically leads to computationally demanding simulations, consuming long periods of processing time. This is mainly due to two factors: first, the computational complexity associated with the density of nodes necessary to accurately discretize the spatial domain and the nature of the FDTD methodology which is based on a leap-frog scheme; second, the hardware and software limitations of the computational resources that are typically used, such as bandwidth constraints or the low

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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http://dx.doi.org/10.1016/j.cpc.2017.08.023
0010-4655/

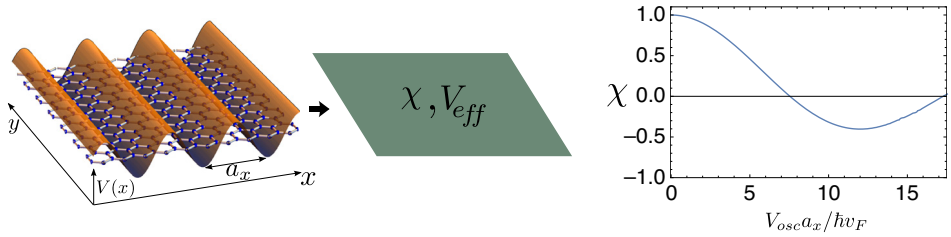

Fig. 1. (a) Graphene superlattice characterized by a sinusoidal electrostatic potential in the microscopic model and the corresponding continuum model where the granular details are homogenized. (b) Anisotropy parameter χ of the homogenized superlattice as a function of the peak modulation amplitude V_{osc}.

number of cores available in central processing units (CPUs) or the available sequential programming models.

The purpose of this work is to develop a framework that enables the fast simulation of the electron wave dynamics in GSLs using either a "microscopic" approach (relying on the two-dimensional massless Dirac equation) or an effective medium formalism wherein the microscopic details of the superlattice are described by some effective parameters. Particularly, we focus on parallelization strategies relying on the C/OpenCL standards to exploit higher throughput performance in heterogeneous multi-GPU environments [20–23]. To this end, we propose two distinct models, namely a simulation concurrency model and a device concurrency model that capture different simulation scenarios. Furthermore, we present a detailed study of a time evolution problem in graphene superlattices with localized scattering centers.

The article is organized as follows. In Section 2 we present a brief overview of the electron wave propagation in GSLs and of the FDTD numerical solution. Section 3 describes the adopted computational procedures and parallelization strategies. The proposed methodologies are applied to study the time evolution of electronic states in a superlattice with localized scattering centers in Section 4. Performance metrics are reported and discussed in Section 5. The article ends with a brief conclusion in Section 6.

2. Graphene superlattices and the electron wave propagation

2.1. Formalism

This section identifies and describes the key steps in the formalization of the equations that govern the behavior of electron waves in graphene-based nanostructures. This method was developed in [15] and establishes the basis of our study.

The propagation of charge carriers in graphene superlattices may be characterized in the spatial and time domains by solving the massless Dirac equation [12]:

$$\hat{H}\psi = i\hbar\frac{\partial}{\partial t}\psi, \tag{1}$$

being $\hat{H} = -i\hbar v_F \sigma \cdot \nabla + V(x,y)$ the microscopic Hamiltonian operator near the K point, V the microscopic electric potential, $\psi = \{\Psi_1, \Psi_2\}^T$ the two component pseudospinor, $v_F \approx 10^6 m/s$ is the Fermi velocity, $\sigma = \sigma_x\hat{x} + \sigma_y\hat{y}$ a tensor written in terms of the Pauli matrices and $\nabla = \frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y}$. In GSLs, the potential V is a periodic function of space. A complex spatial dependence of the potential V can increase the computational effort to an undesired level and even limit the understanding of the relevant physical phenomena. A solution to reduce the complexity of the problem is to use effective medium techniques. It was recently shown that electronic states with the pseudo-momentum near the Dirac K point can be accurately modeled using an effective medium framework [24,25]. Within this approach, the microscopic potential is homogenized and the effective Hamiltonian treats the superlattice as a continuum characterized by some effective parameters [24,25]. For the cases of interest in this work, the effective Hamiltonian is of the form:

$$\left(\hat{H}_{eff}\psi\right)(r) = \left[-i\hbar v_F \sigma_{ef} \cdot \nabla + V_{eff}\right] \cdot \psi\,(r)\,, \tag{2}$$

where $\sigma_{eff} = \chi_{xx}\sigma_x\hat{x} + \chi_{yy}\sigma_y\hat{y}$ and V_{eff} is an effective potential. Moreover, the energy dispersion of the stationary states in the homogenized superlattice can be calculated using [24]:

$$|E - V_{eff}| = \hbar v_F \sqrt{\chi_{xx}^2 k_x^2 + \chi_{yy}^2 k_y^2}, \tag{3}$$

where $\mathbf{k} = (k_x,\ k_y)$ is the wave vector of the electronic state with respect to the K point and E is the electron energy.

Next we characterize the effective parameters χ_{xx}, χ_{yy} and V_{eff} of the effective Hamiltonian of two distinct superlattices.

2.1.1. Anisotropic superlattices

To begin with, we consider 1D-type graphene superlattices described by a microscopic potential with a spatial variation $V(x) = V_{av} + V_{osc}\sin(2\pi x/a_x)$, as shown in Fig. 1. Here, V_{av} is the average electric potential, V_{osc} is the peak amplitude of the oscillations and a_x is the spatial period. These structures have been extensively studied in the literature and can have strongly anisotropic Dirac cones and particle velocities, allowing for the diffractionless propagation of electron waves [5,6,15,25].

The continuum model for the propagation of electrons in these superlattices was thoroughly discussed in [15,24,25]. In particular, in Ref. [24] it was found that the effective parameters of the stratified superlattice satisfy $\chi_{xx} = 1$ and $\chi_{yy} = \chi$. The anisotropy parameter χ depends on the peak modulation amplitude V_{osc} and can be numerically calculated using the approach described in [24]. The explicit dependence of χ on V_{osc} is represented in Fig. 1, and it varies from $\chi = -0.4$ to $\chi = 1$. The latter value corresponds to pristine graphene. The anisotropy ratio determines the (wave packet) electron velocity, which under the continuum formalism is $\mathbf{v} = \frac{1}{\hbar}\nabla_k E = \mathrm{sgn}(E - V_{av})v_F(k_x^2 + \chi^2 k_y^2)^{-\frac{1}{2}}(k_x\hat{x} + \chi^2 k_y\hat{y})$ [15,24,25]. Thus, the value of χ determines the degree of anisotropy and a preferred direction of propagation. In particular, in an extreme anisotropy regime, where the anisotropy ratio vanishes, $\chi = 0$, the group velocity is equal to $v = \pm v_F\hat{x}$, so that the electron waves propagate without diffraction along the x-direction [3,15,26–30]. Thus the electron transport differs in a drastic manner from pristine graphene ($\chi = 1$) wherein the electrons propagate parallel to the quasi-momentum $\mathbf{k}$.

2.1.2. Superlattices with localized scattering centers

Next, we characterize the effective Hamiltonian of a superlattice formed by localized scattering centers, which is modeled by an electric potential periodic in the x- and y-coordinates $V(x,y) = V_{av} + V_{osc}\sin(2\pi x/a_x)\sin(2\pi y/a_y)$ as illustrated in Fig. 2. To the best of our knowledge, this superlattice was not previously discussed in detail in the literature. In this work, it is assumed that $a_x = a_y =$

Please cite this article in press as: M.J. Rodrigues, et al., Simulating electron wave dynamics in graphene superlattices exploiting parallel processing advantages, Computer Physics Communications (2017), http://dx.doi.org/10.1016/j.cpc.2017.08.023.