Modeling Quantum Acceleration of Bloch Waves in Nanowires

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INTRODUCTION

The drift model used in a 'free-flight drift' routine of a Monte Carlo simulation of semiconductor devices is a single band model that does not work well at band crossings or when the energy separation between the bands are small. Applying strong electric fields to semiconductors can induce inter band transitions [1]. This effect becomes prominent in materials such as nanowires where the energy spacing between the bands is small and the bands intercross more frequently across the Brillouin Zone (BZ). Various approaches have been proposed to incorporate carrier transitions between different bands such as the overlap test [2] and the velocity continuity method [3]. Both these methods have a drawback that the transition does not depend on the electric field and is sensitive to the mesh size [4]. Krieger and Iafrate (KI) have developed a set of equations which when solved give the transition probability of a carrier as a function of time under an electric field [5]. The KI method has been applied here to the case of nanowires and the method and results discussed in the following sections.

MODEL

The KI method solves the time dependent Schrodinger equation for Bloch waves under an electric field to give the following set of coupled partial differential equations.

$$i\hbar\frac{\partial C_n(t)}{\partial t} = \varepsilon_n(k(t)).C_n(t) + eE(t) \times \sum_{n'} X_{n,n'}(k(t)).C_{n'}(t) \quad (1)$$

where *E(t)* is the electric field, (*-e*) is the electronic charge and the wave vector *k(t)* is determined by the semi-classical relation,

$$\hbar\frac{\partial k(t)}{\partial t} = -eE(t) \quad (2)$$

The X-matrices are defined as

$$X_{n,n'}(k(t)) = -i\int_{\Omega} u^*_{n,k(t)}(x).\nabla_k u_{n',k(t)}(x).d^3x \quad (3)$$

where Ω is the volume of the primitive cell. The derivative in eqn. 3 is calculated using Rayleigh-Schrodinger perturbation theory as shown in eqn. 4. For degenerate bands the degenerate perturbation theory is used.

$$\nabla_k u_n(k) = \sum_{n',n'\neq n} \frac{\langle u_{n',k}|\partial H/\partial k|u_{n,k}\rangle}{\varepsilon_{n'}(k)-\varepsilon_n(k)} u_{n'}(k) \quad (4)$$

Equation 1 is solved using the 4th order Runge-Kutta method for coupled partial differential equations [6]. Special care is taken to ensure the phases of the X-matrices are continuous across different k-points as noted in [7]. The probability distributions obtained from eqn. 1 are calculated for every k point in the BZ for a given free-flight time step for all possible initial conditions before the simulation starts. The band structure and scattering rates of the nanowires are calculated as shown in [8]. A uniform field Monte Carlo simulation is then run to calculate the energy field characteristics. At the beginning of every free-flight step the carrier's momentum is updated according to eqn. 2. Based on the carrier's initial momentum value and band index the corresponding probability distributions are obtained from the pre-calculated tables and a random number is used to decide the final band index. The carrier is then placed in that band.

RESULTS

The nanowires considered in this study are 3nmx3nm rectangular Si and InAs nanowires along the [100] direction. The band structure of a 3nmx3nm InAs nanowire is shown in Fig.1. At high energies an electron has the chance of getting

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trapped within a band unless it can tunnel to higher bands using the electric field. In Fig.2 we see the difference the quantum acceleration model produces on the average energy of the electrons in a uniform field simulation in a 3nmx3nm InAs nanowire. Without it the electron energy begins to saturate as the carriers are unable to gain sufficient energy from the electric field. In Fig. 3 we see a specific example of a band crossing in the Si nanowire highlighted by the circle. In Fig. 4 the probability of finding an electron in each band is shown after the electron is drifted across the band crossing under an electric field of -100kV/cm. The electron is initially placed in the 9th conduction band.

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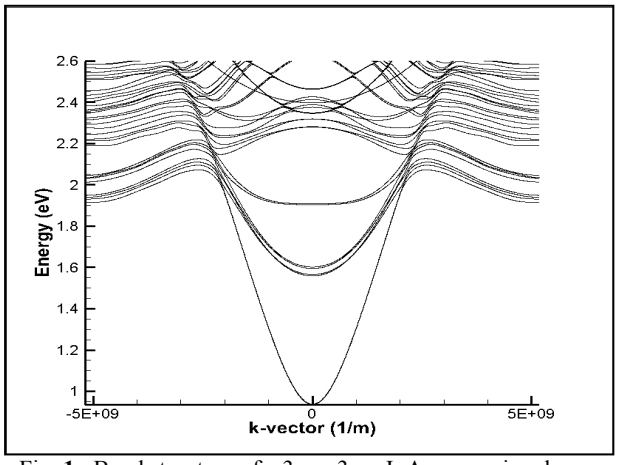

Fig. **1**. Band structure of a 3nmx3nm InAs nanowire along the 100 direction.

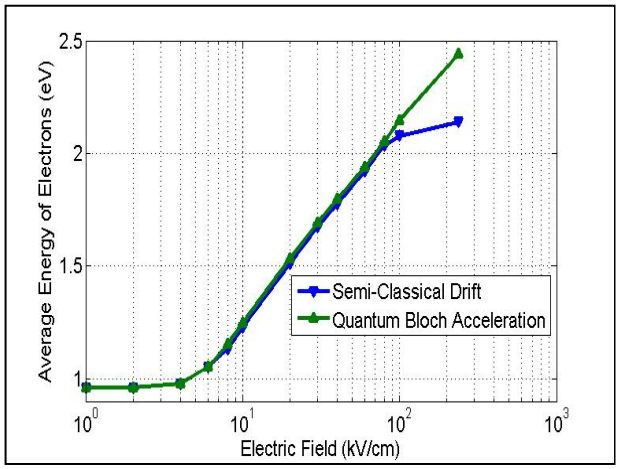

Fig. 2. Average energy of the electrons in a uniform field simulation with the traditional (semi-classical) drift model (blue) and with the quantum acceleration model (green) as a function of electric field. This is for a 3nmx3nm InAs nanowire.

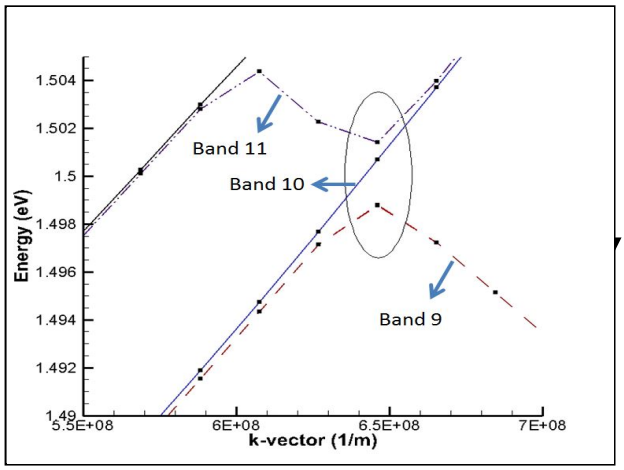

Fig. 3. Band structure crossing for a 3nmx3nm Si nanowire along the 100 direction. The black dots represent the discrete eigenvalues obtained from the eigensolver.

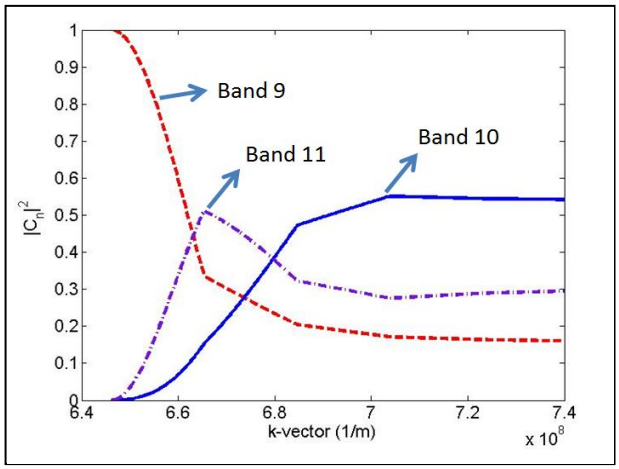

Fig. 4. Probability distribution of the electron as it drifts across the band crossing under an electric field of -100kV/cm.