Monte Carlo simulation of multi-band carrier transport in semiconductor materials with complex unit cells

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Abstract

In a traditional Monte Carlo (MC) model the carrier preserves its band identity during the free flight between scatterings. However, this assumption may not be valid in semiconductor materials with complex unit cell. A new model is needed where the traditional way to use classical equations during the free flight between scattering is replaced by a fully quantum mechanical model of the Bloch carrier dynamics between scattering events. In this work we present such a model along with simulated results of the hole initiated impact ionization coefficients of 4H-SiC.

1 Introduction

Silicon Carbide is a semiconductor that recently has attracted a lot of attention due to its high breakdown field and high thermal conductivity. These characteristics make it a very promising semiconductor material for high field and high temperature applications. 4H-SiC is a hexagonal SiC polytype with 8 atoms in the unit cell. This level of complexity in the unit cell introduces new challenges in the area of full band Monte Carlo (MC) simulation. An important feature in the 4H-SiC band structure is the large number of bands within a limited energy range (see Fig. 1), which means that interband tunneling is significant at high electric fields. This is especially true for the valence band where the multi-band picture is very pronounced even at low energies. In order to model the hole transport in 4H-SiC a fully quantum mechanical transport model is needed. Krieger and Iafrate have proposed a theory for the time evolution of Bloch electrons in a homogeneous electric field [1]. This theory has been used to develop a fully quantum mechanical Monte Carlo simulator (QM-MC), where both scattering and drift are treated as quantum mechanical processes. In order to evaluate the importance of this type of model we have simulated the hole initiated impact ionization coefficient of 4H-SiC and compared the results with two independent measurements.

2 New numerical model for the carrier dynamics

In the theoretical framework developed by Krieger and Iafrate [1] the time development of the probability $|\alpha_n(t)|^2$ to be in band n for a Bloch electron moving in a homogenous electric field can be found by solving the following system of linear differential equations

$$\frac{d\alpha_n(t)}{dt} = \frac{1}{i\hbar}\sum_{n'}\alpha_{n'}(t)FX_{nn'}(\bar{k}(t))\exp\left(\frac{i}{\hbar}\int_0^t\left[E_n(\bar{k}(t')) - E_{n'}(\bar{k}(t'))\right]dt'\right) \quad (1)$$

F is the force due to the electric field and $E_n(\boldsymbol{k})$ is the energy dispersion for band n at wave vector **k**. We have dropped the vector notation for $X_{nn'}$ and F, since the motion in k-space is parallel to the force. If $\alpha_{n'}=\delta_{nn'}$ at time $t=0$ we can interpret $|\alpha_n(t)|^2$ as the probability of changing band from band n to band n' after a drift t. Assuming an electric field applied in the c-axis direction (k_z direction) then the quantity $X_{nn'}(\boldsymbol{k})$ can be defined as

$$X_{nn'} \equiv \frac{1}{i}\int_{cell} U^*_{nk}\frac{\partial}{\partial k_z}U_{n'\bar{k}}\,dr^3 \approx \frac{1}{i|\Delta\bar{k}|}\begin{cases} I_{nn'}(\bar{k},\bar{k}+\Delta\bar{k}) & , \quad n\neq n' \\ i\cdot imag(I_{nn'}(\bar{k},\bar{k}+\Delta\bar{k})) & , \quad n=n' \end{cases} \quad (2)$$

U_{nk} is the periodic part of the Bloch wave function and the integration is performed over the unit cell. It is possible to use the overlap integral of the wave functions obtained from the empirical pseudopotential band structure calculation to derive $X_{nn'}(\boldsymbol{k})$. The numerical approximation used to calculate $X_{nn'}(\boldsymbol{k})$ from the overlap integral $I_{nn'}(\boldsymbol{k}, \boldsymbol{k'})$ is also presented in equation (2).

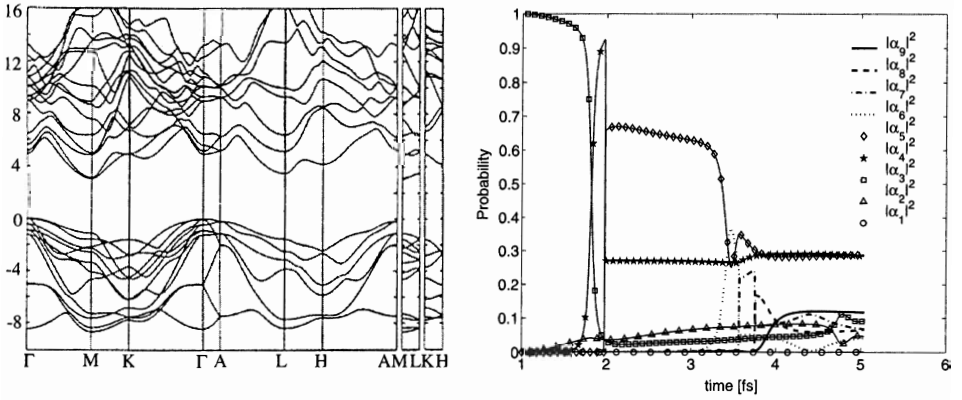

Fig. 1. Left: Empirical pseudopotential band structure in 4H-SiC.
Right: Typical time evolution of the probability amplitudes.

The expression (2) in the case of n equal to n' ensures the condition that X_{nn} should be real [2].

There are some practical issues that need to be considered to extract $X_{nn'}$ from the band structure. $X_{nn'}$ should be used for integration, which means that all values need to have the same phase reference. Many eigenvalue solvers provide results with an

arbitrary phase factor. The arbitrary phase factor is different at different bands and k-points and has to be removed before $X_{nn'}$ can be extracted using equation (2). The EISPACK eigenvalue solver [3] used in this work provides an arbitrary phase factor that is easy to predict and remove.

Equation (1) can be solved using a Runge-Kutta integration scheme. In Fig. 1, the probability density for a hole initially in band 3 is plotted as a function of time for a drift trajectory parallel to the c-axis. During the drift the probability to be in different bands vary drastically and at the end of the drift the hole can emerge into any one of the nine possible bands albeit with different probabilities.

The primary difference between the current technique and standard MC is that during the course of the drift, the carrier cannot be definitively assigned to a specific band. As such, at different time intervals during the drift, the magnitude of the physical quantities such as scattering time, etc. must be determined based on the probability densities. To this end, we use the simplest formulation given as,

$$A(\bar{k}(t)) = \sum_{n=1}^{N} \left|\alpha_n(t)\right|^2 A_n(\bar{k}(t)) \tag{3}$$

to determine $A(\boldsymbol{k}(t))$, the value of the desired quantity. $A(\boldsymbol{k}(t))$ is found by summing its value in each band, $A_n(\boldsymbol{k}(t))$ weighted by the probability density, $|\alpha_n(t)|^2$ over all N possible bands. The time between scatterings is thus determined terminating the free flight drift. The band index is then determined stochastically based on the probability densities and a subsequent scattering event and final state is selected for the carrier from this initial band.

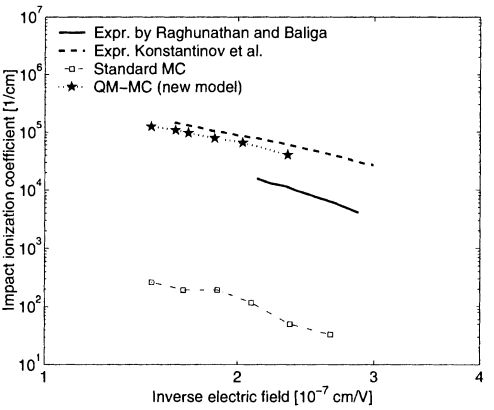

Fig. 2. Comparison between experimental and simulated hole initiated impact ionization coefficients in 4H-SiC

$X_{nn'}$ is a rapidly varying function of the k-vector and a very dense mesh has to be used in the discretization scheme. In this work we are considering transport in a homogenous electric field directed parallel to the c-axis in 4H-SiC. This allows us to reduce the storage requirements by considering only one component of the $X_{nn'}$ vector.

3 Monte Carlo simulation

The full band MC model uses numerically calculated k-dependent scattering rates. The scattering mechanisms are; acoustic phonon scattering, polar and nonpolar optical phonon scattering, ionized impurity scattering and impact ionization. The impact ionization transition rates have been calculated following the approach presented in Ref [4]. There are two independent measurements of the hole initiated impact ionization coefficients in 4H-SiC [5][6]. In Fig. 2 we have compared results from our new MC model with these two measurements. We have also included simulation results obtained using the standard full band MC approach with a classical model for the carrier dynamics. The new model provides results that are similar to the experimental data, while the standard MC model gives results that are almost three orders of magnitude lower. This demonstrates the importance of a fully quantum mechanical dynamic equation in MC simulation of charge transport in 4H-SiC. This conclusion can be extended to other semiconductors with a band structure containing a significant amount of band intersections.

4 Conclusion

A new approach to simulate the carrier transport in semiconductors with complex unit cell and band structure is presented. In the new MC model the traditional way of using classical equations during the free flight between scattering has been replaced by a fully quantum mechanical dynamic equation. The quantum mechanical model allows carriers to tunnel between bands during the drift. In the case of hole transport in 4H-SiC this tunneling is very strong and it enhances the carrier heating drastically. The simulated hole initiated impact ionization coefficients increase by three orders of magnitude when the new model is employed yielding results that are in good agreement with the presently available experimental data.

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