

# Scattering in Si-Nanowires – Where does it matter?

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**Abstract** – Electron transport is computed in 3nm Si nanowires subject to incoherent scattering from phonons. The electronic structure of the nanowire is represented in an atomistic  $sp^3d^5s^*$  tight binding basis. Phonon modes are computed in an atomistic valence force field rather than a continuum deformation potential. Atomistic transport and incoherent scattering are coupled through the non-equilibrium Green function formalism (NEGF) in our new OMEN simulator. Energy loss due to phonon emission is shown to lead to a resistive potential drop in the emitter of the nanowire. Phonon absorption is shown to increase the current in a band-to-band-tunneling configuration.

## I. INTRODUCTION

Nanowires represent the ultimate 3D scaling limit of a charge-based transistor. The possibility of close gate proximity in 3 or even 4 sides along the transport direction of the nanowire affords a very strong gate control, possibly enabling the usage of smaller supply voltages. A variety of different material systems and geometrical configurations are being explored experimentally and theoretically. Simulation models that have been carefully calibrated against experimental data promise a better understanding of these devices and possibly the reduction of experimental costs. For the comprehensive study of electronic states and carrier transport at the nano-scale we have developed the NEMO and OMEN tool suite over the past 15 years [1-5].

*Need for Atomistic Nanowire Representation:* Semiconductor device modeling is typically performed within the assumption of an effective mass description of the material that is widely employed in conjunction with classical transport models as well as quantum transport models. The need for an atomistic model was demonstrated for electrons [6, 7] and for holes [8] in Si with a “simple” top of the barrier (ToB) model which provides good insight into the importance of bandstructure on crystal orientation, confinement, and electrostatic potentials. The ToB model computes the dispersion in the wire cross section, neglects the tunneling through the gate potential barrier, and determines the top of the barrier potential through capacitive considerations. Atomistic full 3D models are possible but are typically limited to nanowires with less than 2nm in diameter. Efficient numerical algorithms and the availability of parallel computers have made the simulation of more practical devices of up to 10nm diameter possible [3, 9]. With the availability of a full 3D atomistic model the “simple” ToB model could be calibrated for several nanowire configurations [10]. The two models agree well when the device length exceeds the wire diameter by a factor of 5. Shorter wires exhibit significant source-to-drain tunneling.

## II. METHODOLOGY

Here a full band atomistic  $sp^3d^5s^*$  TB model is implemented in the new simulator OMEN. Incoherent scattering from phonons is

treated in the NEGF formalism. All confined phonon modes are treated through an atomistic representation with a valence force field (VFF) rather than a continuum deformation potential model. Atomistic full-band simulations are computationally very intensive, requiring up to tens of thousands of processors on today’s most powerful computers. Details of the methodology are given in reference [11].

OMEN can handle a variety of different device geometries and materials as depicted in Fig. 1. We consider a 3nm circular Si nanowire with a gate length of 15nm and 1nm oxide thickness.

## III. RESULT AND DISCUSSION

*Resistive Potential Drop in the Emitter:* Small Si nanowires have been extensively investigated under the assumption of ballistic transport. The inclusion of incoherent scattering into an atomistic model had been considered by many device engineers computationally prohibitive. Now with the recent developments of OMEN we can compare a completely coherent simulation against one that includes incoherent phonon scattering will all phonon modes. Indeed we can actually “look” at the resistive potential drop in the emitter (Fig. 2b). The energy-resolved current density plot indicates the energy loss of the electrons in the emitter of the wire. The current density shows spectral features that can be traced to the available phonon modes of the device [11]. Scattering reduces the current as one would expect from resistive losses (Fig. 2c).

*Phonon absorption can enhance current flow:* Typically one thinks of phonon scattering being a source of current reduction resulting in an increased resistance. There are, however, device configurations and operational conditions in which phonons are needed to provide additional transition paths through a device. In particular it is well understood that band-to-band tunneling is strongly enhanced in Silicon by phonon scattering. In Ref. [12], for example, phonon scattering was implemented in a full-band model in a 1D geometry for a single phonon event. Good agreement with experimental data could be achieved demonstrating the capability to model phonon-scattering in full-band in Si. Here, we show in the case of a p-i-n band-to-band-tunneling configuration how phonon absorption indeed can enhance the current flow through a Si nanowire (Fig. 3). Phonon absorption is needed to lift electrons from the valence band into the conduction band.

## IV. CONCLUSIONS

Nanowire transport can be modeled in a fully atomistic representation with the new OMEN tool. Incoherent scattering from all phonon modes can be included through the NEGF formalism.

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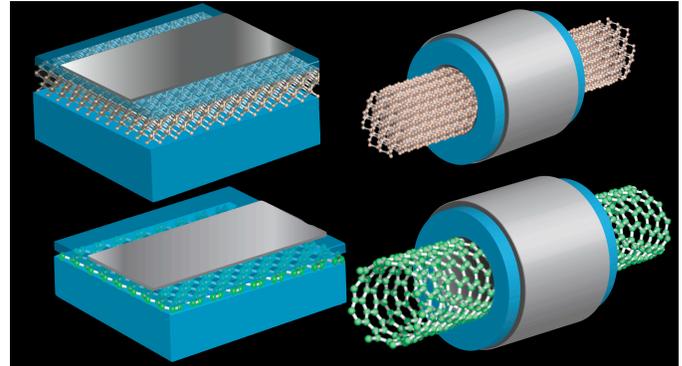


Fig. 1. Possible OMEN atomistic device geometries, ultrathin bodies, nanowires, grapheme, and carbon nanotubes.

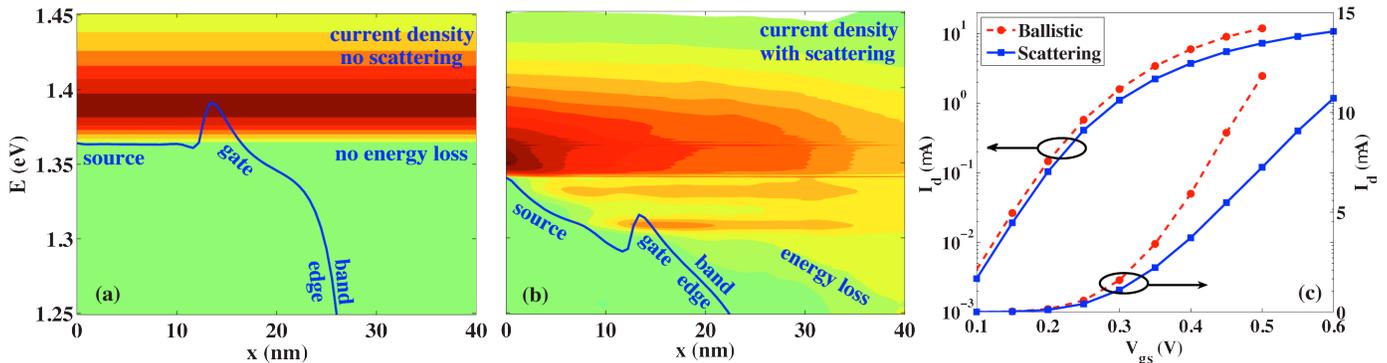


Fig. 2. (a,b) Current density in a 3nm Si nanowire. (a) fully coherent. (b) with incoherent scattering. Electrons experience an energy loss and there is a distinct resistive potential drop in the source. (c) Current voltage characteristics with and without scattering. Scattering reduces the current flow.

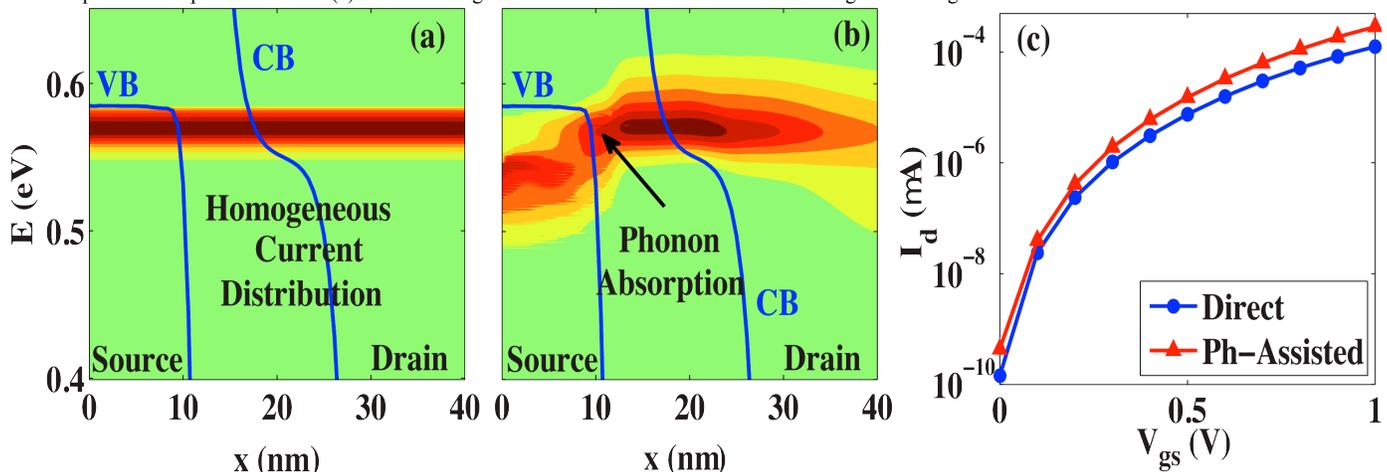


Fig. 3. (a,b) Current density in a 3nm p-i-n nanowire. (a) fully coherent. (b) with incoherent scattering. Phonon absorption increases the current flow in the band to band tunneling configuration. (c) current voltage characteristics.