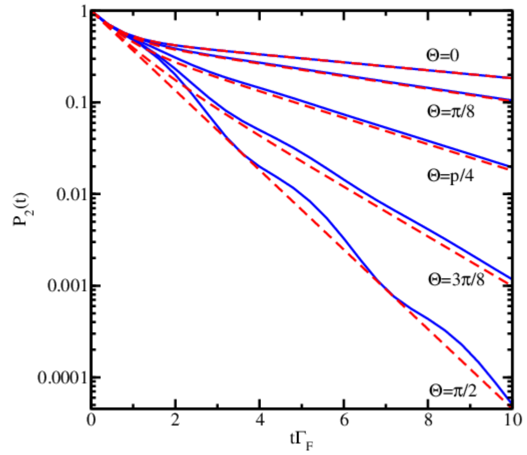

Fig.5 Probability distribution of escape times for ω_L=2Γ_F, |**p**|=0.9 compared to those computed with the method from [2].

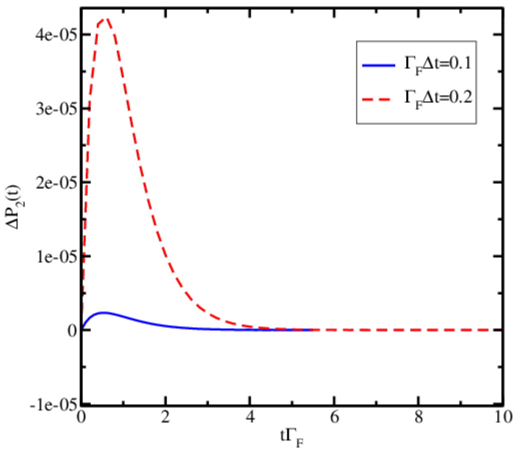

Fig.6 Validation of the numerical rates for two different time steps by comparing with the analytical results from [2] for $\Theta = 0$.

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Full band Monte Carlo simulation of high-field transport in si nanowires

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The effect of collision broadening on the number of impact events has previously been studied in bulk materials. It was shown that incorporating collision broadening increases the number of impact events in the bulk [1]. In this paper, we study the effect of collision broadening in nanowires, where it is expected to have more significance due to the 1D nature of the density of states. In this initial study, a simple Lorentzian broadening is employed and its effects on the velocity field and impact ionization events are studied. A full band impact ionization rate for nanowires is also presented for the first time within the tight binding scheme.

The band structure of the Si nanowires along the [100] direction is calculated according to the empirical tight binding method (TB) [2]. The deformation potential scattering rates are calculated using Fermi's golden rule from the TB coefficients using the method outlined in [3]. At high electric fields multiband tunneling during the free-flight process becomes important [4]. This is taken into account by solving the Krieger and Iafrate equations using the Magnus expansion method [5]. The impact ionization rate is derived for nanowires within the TB scheme and is given by eqn. (1) $k_{1,n}$ represents the high energy electron/hole impacting with a valence band electron/conduction band hole, $k_{4,m}$ creating two new electrons/holes, $k_{2,n'}$ and $k_{3,m'}$.

$$W_{II}\left(k_{1,n},\Delta k_{2,n'}\right)=\frac{e^4}{\varepsilon^2\left(2\pi\right)^3\hbar}\times\int_{E_{min}}^{E_{max}}\sum_{k_3 m,m'}\left|F_{\substack{n,n'\\m,m'}}\left(k_1,k_2,k_3,k_4\right)\right|^2\times\left[JDOS_{m,m'}\left(k_4,k_3\right)\right]DOS_{n'}\left(k_2\right)dE_{n'}\left(k_2\right) \quad (1)$$

where the overlap integral is given by

$$F_{\substack{n,n'\\m,m'}}\left(k_1,k_2,k_3,k_4\right)=\sum_{\mu,\nu}e^{iq_x\left|\tau_\mu-\tau_\nu\right|}\int_{q_t}\frac{J_0\left(q_t a_{diff}\right)}{q_x^2+q_t^2}\times C_{n,\mu}\left(k_1\right)C^*_{n',\mu}\left(k_2\right)C_{m,\nu}\left(k_4\right)C^*_{m',\nu}\left(k_3\right)q_t dq_t \quad (2)$$

and the joint density of states is

$$JDOS_{m,m'}\left(k_a,k_b\right)=\frac{1}{\left|\frac{\partial E_m\left(k_a\right)}{\partial k_b}-\frac{\partial E_{m'}\left(k_b\right)}{\partial k_b}\right|} \quad (3)$$

$q_x=(k_1-k_2)$, τ_μ is the atom position, $a_{diff}=\sqrt{\left(\tau_{\mu,y}-\tau_{\mu',y}\right)^2+\left(\tau_{\mu,z}-\tau_{\mu',z}\right)^2}$

and $C_{i,j}\,(k)$ are the tight binding coefficients.

The calculation of the overlap integral given by eqn. (2) is computationally very expensive. It can be replaced with a constant overlap integral which greatly reduces the number of computations while still being fairly accurate as shown in Fig.1 and Fig.2, though the effect of the approximation on the anisotropy of the impact ionization rates is unclear.

As an initial study of the effect of collision broadening on the high field properties of Si nanowires, the final energy after a scattering event is governed by a Lorentzian distribution rather than a delta function. The width of the Lorentzian distribution is given by the total scattering rate at that energy [6].

The nanowires considered in this study are 2nm x 2nm rectangular Si nanowires along the [100] direction. The effect of adding the simple collision broadening on the velocity- field curves is shown in Fig.3. The addition of collision broadening reduces the mobility and the peak velocity. In Fig.4 the energy distribution of electrons at an electric field of 750 kV/cm after they have reached steady state is shown. When collision broadening is included, the electrons are able to reach much higher energies as shown in the figure.

This increase in the energy distribution leads to a significant increase in the number of impact events occurring as shown in Fig. 5. Therefore the correct treatment of collision broadening is important to properly understand the role of impact ionization at high electric fields in nanowires.

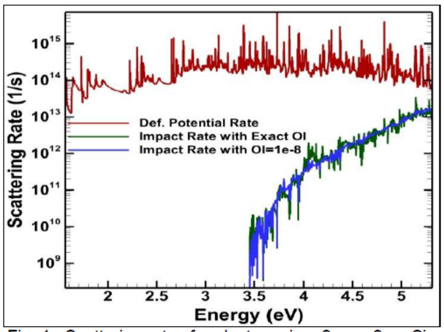

Fig. 1. Scattering rates for electrons in a 2nm x 2nm Si nanowire. Comparison between the exact impact ionization rate and the rate calculate with a fixed overlap integral of 10^{-8}.

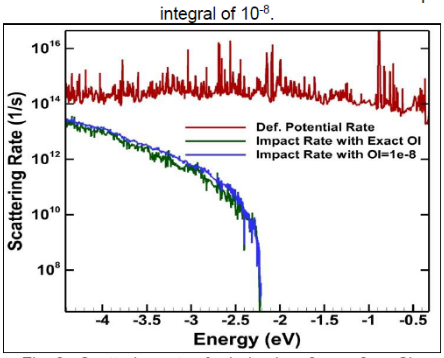

Fig. 2. Scattering rates for holes in a 2nm x 2nm Si nanowire. Comparison between the exact impact ionization rate and the rate calculate with a fixed overlap integral of 10^{-8}.

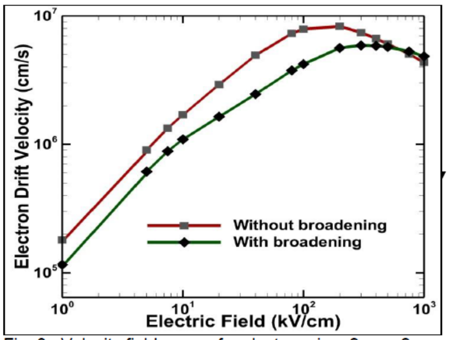

Fig. 3. Velocity field curves for electrons in a 2nm x 2nm Si nanowire with and without Lorentzian broadening.

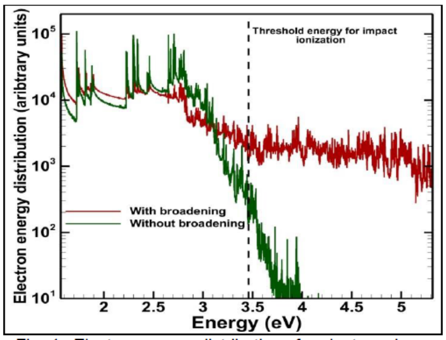

Fig. 4. Electron energy distributions for electrons in a 2nm x 2nm Si nanowire at 750 kV/cm with and without Lorentzian broadening.

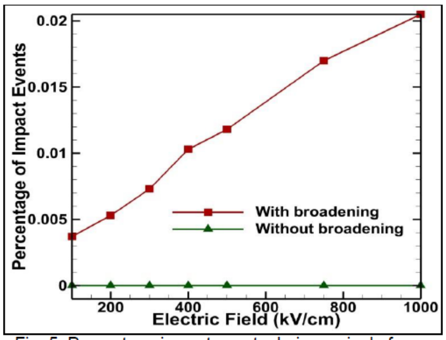

Fig. 5. Percentage impact events during a single free-flight duration of electrons in a 2nm x 2nm Si nanowire with and without Lorentzian broadening.

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