Electronic and Thermal Transport in Sinusoidal Semiconductor Nanowires

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In recent years, there has been a growing interest in exploring semiconductor nanowire as viable candidate for applications in efficient thermoelectric energy conversion [1]. While the dimensionless thermoelectric figure of merit ($ZT = S^2GT/\kappa$) of bulk silicon is around 0.01, silicon nanowires show an enhancement of ZT by a few orders of magnitude [2]. High ZT may be achieved through an approach called 'electron-crystal, phonon-glass'. It is also expected that semiconductor nanowires with nano-engineered geometries can draw more efficient phonon surface scattering as the diameter is reduced to below 50 nm [3]. The corresponding drop in thermal conductivity may provide an enhancement of ZT if the electronic transport is not affected by surface scattering.

In this study, our goal is to investigate trade-offs to maximize the figure of merit ZT in semiconductor wires with non-uniform shape. For instance, we will consider sinusoidal wires, as schematically depicted in Fig. 1, which may be candidates to realize a phonon blockade as discussed in [4] without degrading appreciably the electronic current. Various solutions of electronic quantum transmission for silicon bars with sinusoidal undulations are shown in Figs. 2, 3, and 4 including a comparison with straight bars of the same cross-section (Fig. 2). The transmission coefficient is directly proportional to the wire resistivity due to the scattering mechanism. The 3D conduction channel is modeled by a 1D tight binding chain, and the quantum nature is accounted by solving the Schrödinger equation for each cross section in the transverse direction [5]. Silicon nanowires with length of 30nm and cross-sectional width of 6nm and 10 nm are considered; several numbers of undulation peaks (N) and heights (H) define the shape of undulation within the fixed length (L) by changing periods of undulation. The nanowire undulations directly affect the resistivity particularly at higher carrier energy. However, for the narrower wire, one can see that increasing the number of undulations only decreases the transmission coefficient in a small way.

An atomistic Green's function (AGF) method based on a quantum mechanical description of the phonon energy distribution has been used to simulate phonon transport through nanowires [6]. The AGF method is benchmarked to investigate the degraded phonon transport through sinusoidally undulated silicon nanowires. Figure 5 shows a comparison of phonon transmission coefficients of the undulated silicon bar with the straight bar. The total transmission coefficients over the frequency region are 430 and 386 (a.u) for the straight and undulated bars, respectively, and a reduction of heat flux is expected with the drop in phonon transmission coefficient.

We plan to show comprehensive results illustrating possible trade-offs to optimize the thermoelectric figure of merits in Si and GaAs sinusoidal nanowires with various parameters.

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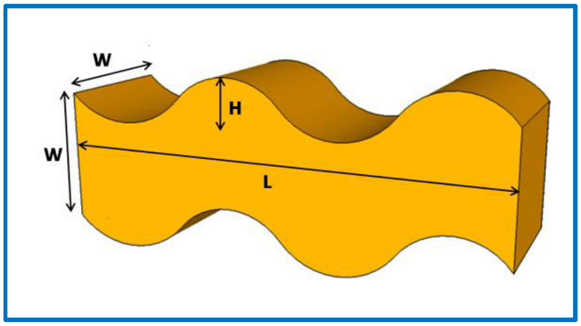

Figure 1. 3D Model of a silicon nanowire with sinusoidal undulation with its geometrical parameters.

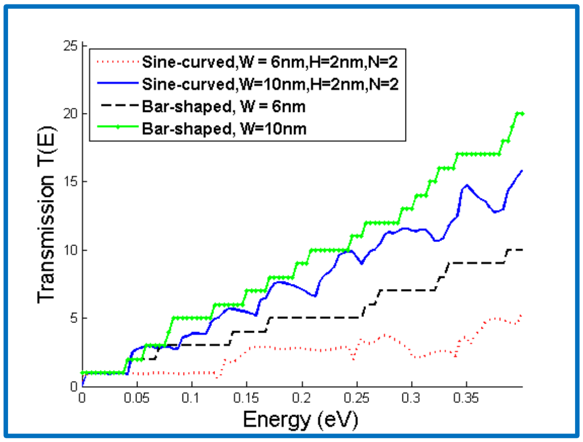

Figure 2. Comparison of sine-curved NWs with uncurved bar-shaped NWs, W=6, 10nm.

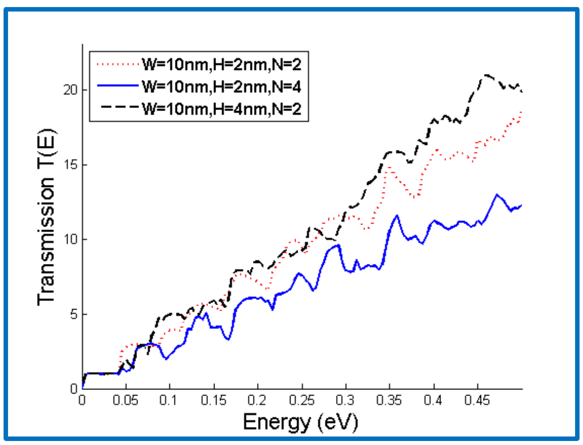

Figure 3. Total transmission coefficient of sine-curved silicon nanowires for varying geometrical parameters. Effect of the peak with varying heights and numbers.

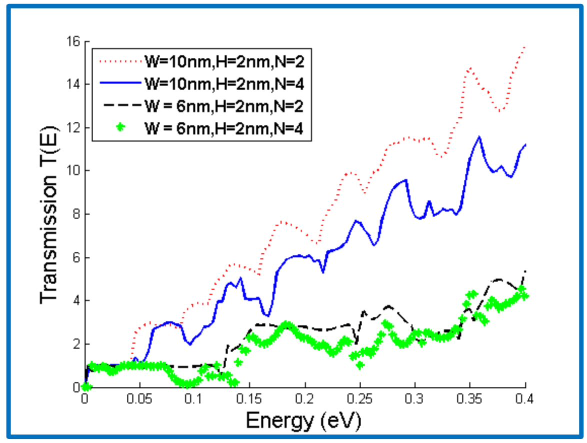

Figure 4. Total transmission coefficient of sine-curved silicon nanowires. Effect of varying width and the number of peaks.

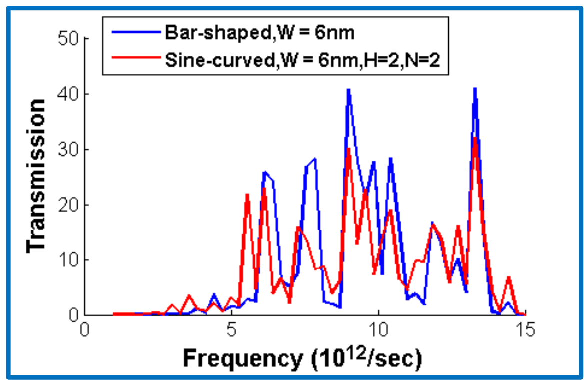

Figure 5. Phonon transmission function of a straight silicon nanowire and an undulated silicon nanowire with W = 6 nm.