# Modeling Thermal Transport in Rough Silicon Nanowires with Phonon Monte Carlo

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Intentionally roughened silicon nanowires show great promise as thermoelectric materials [1]. In general, good thermoelectric materials have high electrical conductivities and low thermal conductivities. Although bulk silicon is a poor thermoelectric material, the rough surfaces of nanowires can drastically lower the thermal conductivity ($\kappa$) without a proportionally large decrease in electrical conductivity. Experiments have shown that the properties of the surface, such as the RMS roughness and correlation length, strongly affect $\kappa$ [1].

A popular model for phonon surface scattering treats the rough surfaces as flat boundaries that diffusely scatter incident phonons [2]. This model predicts a lower bound on $\kappa$, known as the Casimir limit. However, recent measurements have found that silicon nanowires can have thermal conductivities below the Casimir limit [3], necessitating a new model for phonon surface scattering.

Phonon Monte Carlo (PMC) is a technique to solve the Boltzmann Transport Equation for phonons [4], [5]. PMC is an excellent tool for investigating the effects of surface scattering. This method can simulate silicon nanowires of the sizes commonly used in experiments (around 100 nm). We have expanded the PMC method to allow for randomly-generated, real-space roughness (Fig 1) [6].

Rough surfaces allow phonons to become temporarily "stuck" in the wires' crevices (Fig. 2), which can cause lower thermal conductivities than those predicted by the models that treat the surface as flat. Additionally, in our simulations, we can vary the RMS roughness, correlation length, and autocorrelation function (ACF) of the roughness.

Here, we will present the results of our simulations of silicon nanowires with 70 nm width at 300 K. The RMS roughness, correlation length, and ACF have a strong effect on $\kappa$. By varying these parameters, our simulations can produce thermal conductivities below the Casimir limit. These results are in line with experiments, which find that increasing the RMS roughness and decreasing the correlation length can result in thermal conductivities below the Casimir limit. Additionally, changing the ACF from Gaussian to exponential can greatly affect $\kappa$ even when holding the RMS roughness and correlation length constant (Figs. 3 and 4). The differences between thermal conductivities obtained for different ACFs can be seen in Fig. 5. The exponential ACF produces much more short-scale roughness even though the RMS roughness and correlation length are the same for both curves.

## ACKNOWLEDGEMENTS

This work was supported by the DOE, grant No. DE-SC0008712 (primary support) and by the NSF, grant No. 1201311 (partial support).

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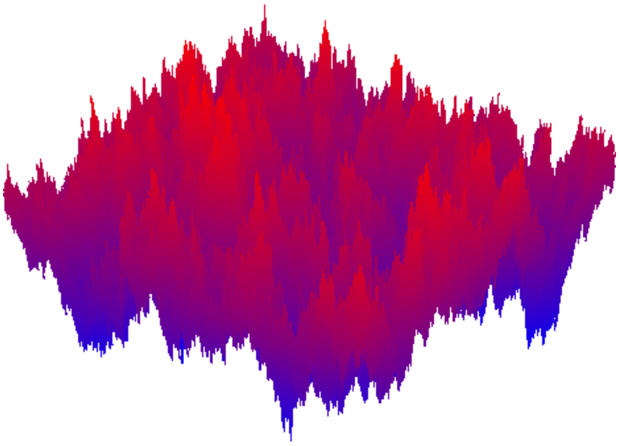

Fig. 1. An example 3D rough surface with a exponential ACF.

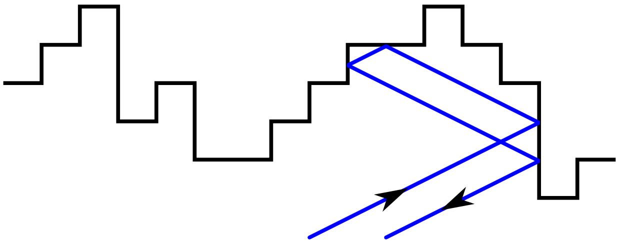

Fig. 2. An example surface and a possible path for a phonon. In addition to changing the phonon's direction, real space roughness allows phonons to become temporarily "stuck" in crevices, effectively slowing their progress through the wire.

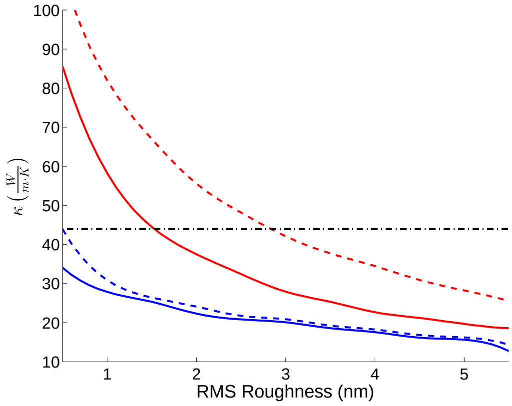

Fig. 3. Thermal conductivity as a function of RMS roughness. The red and blue curves correspond to Gaussian and exponential ACFs, respectively. The dashed and solid lines are for 12 and 2 nm correlation lengths, respectively. The black dash-dot curve is the Casimir limit. As expected, higher RMS roughness leads to lower $\kappa$.

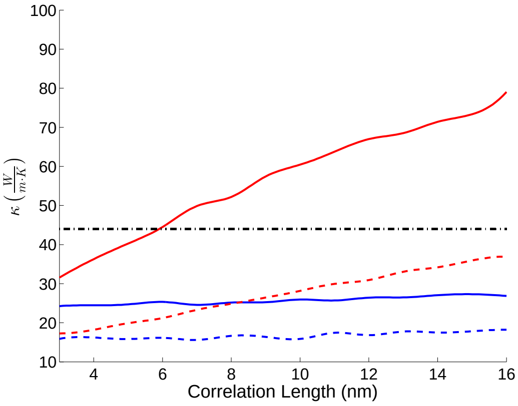

Fig. 4. Thermal conductivity as a function of correlation length. The red and blue curves correspond to Gaussian and exponential ACFs, respectively. The dashed and solid lines are for 4.5 and 1.5 nm RMS roughness, respectively. The black curve is the Casimir limit. Simulations with a Gaussian ACF show $\kappa$ decreasing with correlation length. However, this effect is much less pronounced with exponential ACFs since they have lots of short-scale roughness even for large correlation lengths.

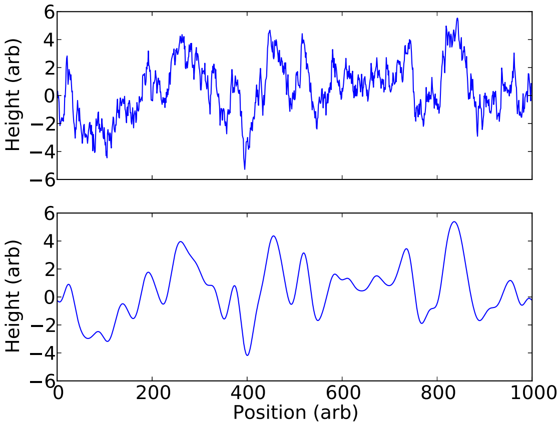

Fig. 5. Example 1D rough, random surfaces generated from exponential (top) and Gaussian (bottom) ACFs. Both curves have the same RMS roughness and correlation length (4 and 25 units, respectively) and share the same large-scale features, which have sizes similar to the correlation length. Additionally, the surface generated from the exponential ACF has much more short-scale roughness, resulting in lower thermal conductivities.