# Atomistic Modeling of the Thermoelectric Power Factor in Ultra-scaled Silicon Nanowires

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**Abstract: Dimensional scaling provides an alternative route to improve the thermoelectric figure of merit (ZT) by the reduction of the lattice thermal conductivity($\kappa_l$). However, this method is reaching the scaling limit. Further improvement in ZT can be achieved by improving the thermoelectric power-factor ($S^2G$), the numerator of ZT. In this work we study this part of ZT using a combination of semi-empirical Tight-Binding method and Landauer approach. We study the effect of cross-sectional confinement, wire orientation and uniaxial strain on the power-factor (PF). It is found that any improvement in PF is only achieved for wires with cross-section size less than 6nm x 6nm.**

**INTRODUCTION:** Thermoelectric conversion efficiency is measured using the dimensionless Thermoelectric Figure of Merit (ZT) [1],

$$ZT = \frac{S^2GT}{(\kappa_l + \kappa_e)} \qquad (1)$$

where S, G, $\kappa_l$ and $\kappa_e$ are the Seebeck coefficient, electronic conductance, lattice thermal conductivity and electronic thermal conductivity respectively. In the past it has been shown that dimension scaling provides a good way of improving ZT beyond 1 by dimensional scaling [2] which suppress the phonons (reducing $\kappa_l$). Recent works [3] show that Silicon nanowires (SiNW) can be used as viable thermoelectric materials. However the thermal conductivity reduction has reached a scaling limit. A recent experimental work [4] shows that further improvement in ZT can be attained by improving the thermoelectric Power-factor (PF = $S^2G$).

**METHODOLOGY:** Modeling S and G for SiNW requires a fundamental understanding of the electronic structure. Wire orientation, cross-section shape and size and geometrical confinement strongly influence the wire dispersion E(k). An atomistic 10 band sp3d5s* semi-empirical Tight-binding (TB) model [5] is used which properly represents the SiNWs below 5~6nm[6]. The S and G are calculated using Landauer's method [7] from SiNW E(k). The 'method of mode counting' is utilized for the calculation of S and G that is outlined in detail in Ref.[8].

In E(k) calculation all the wire surfaces are hydrogen passivated. We denote X as the transport direction and Y-Z as the wire confinement directions. SiNW with cross-section size from 2nm x 2nm till 14nm x 14nm are simulated with sub-bands varying from 30 to 500 respectively, needed for the proper calculation of S and G.

**RESULTS:** The projected atomic locations in the unit cell for three SiNW orientations are shown in Fig.1. The effect of cross-section confinement direction is reflected in the E(k) (Fig.2). For <100> wires Y and Z confinement are the same, however, for <110> and <111> wires Y-Z confinement changes the valleys which are occupied first, which changes the DOS of the system and S and G in turn.

Effects of confinement and asymmetry in the Seebeck coefficient are captured in Fig.3. <100> wires show symmetric S for both W and H confinement. Wires below 5nm x 5nm show higher S. For <110> the asymmetry is more pronounced. It is more beneficial to confine the device along the height (Y) than width. <111> wires also show asymmetry in S for confinement.

The maximum PF (PFmax) shows significant improvement only for wires with cross-section dimension below 6nmx6nm for all orientations (Fig.4a).<111> shows the best PF. The S value at PFmax is almost the same for all the wires (Fig.4b), however, the G value shows improvement below 6nm (Fig.4c), with <111> being the best which explains the PFmax trend.

Compressive uniaxial strain in SiNW improve the PF for n-type SiNW (Fig.5). 1% compressive strain improves the PF by ~1.14X in 4nmx4nm circular SiNW over the unstained case. However, p-type carriers show no improvement in the PF with uniaxial strain (Fig.5). ZT calculated using a $\kappa_l$ of 2W/mK [9] shows an improvement of ~1.25X with compressive strain for 4nmx4nm SiNW(Fig.6)

**CONCLUSIONS:** SiNWs below 6nmx6nm can serve as good candidates for high PF material with <111> as the best. Compressive uniaxial strain can enhance both the PF and the ZT for n-type devices significantly as predicted by atomistic modeling. Confinement direction plays a vital role in obtaining high S value in SiNWs.

**References:** **[1]** A V. Ioffe et. al, Dokl. Akad Nauk SSSR 98 , 5, 1954. **[2]** G. Mahan and J. O. Sofo, Proc. Nat. Acad. Sci. 1996 **[3]** Hochbaum et. al, Nature, 451, 2008. **[4]** J.P. Heremans, Science, 321, 2008. **[5]** Klimeck et. al CMES, 3, 2002, **[6]** Jing Wang et.al, IEDM, 2004. **[7]** R. Landauer, IBM J. Res. Develop. 957 **[8]** C.Jeong et. al, JAP, 107, 2010. **[9]** N. Mingo et. al, Nanolett. 2003.

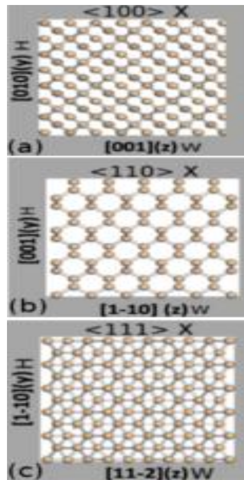


**Fig. 1**. Unit cell structures for Silicon nanowires. **(a)** <100>(X) Y=[001], Z =[0-10] **(b)** <110> (X) ,Y =[001], Z=[1-10] and **(c)** <111>(X) Y=[1-10], Z=[11-2] . Dots represent the atoms.

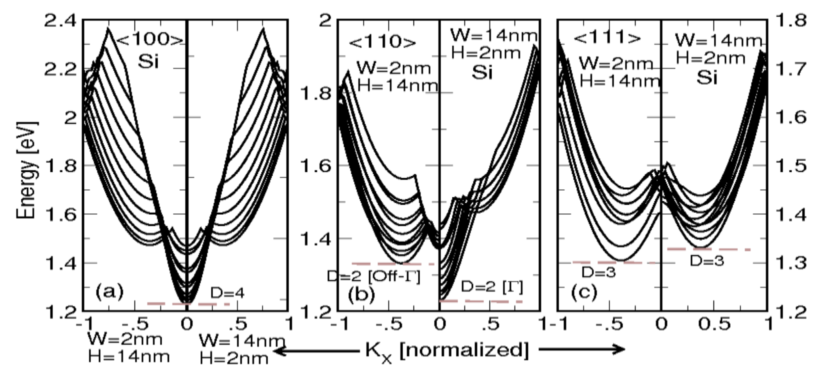


**Fig. 2**. Effect of cross-section confinement on the nanowire E(k). For each wire X is the transport direction and Y (Height) and Z (Width) are the confinement directions.**(a)** <100>(X) **(b)** <110> (X) and **(c)** <111> (X) oriented wires.. For <100> wires Y and Z confinement are similar as reflected from the symmetric E(k). For <110> and <111> wires confinement along Y and Z directions are different due to different atomic arrangements.

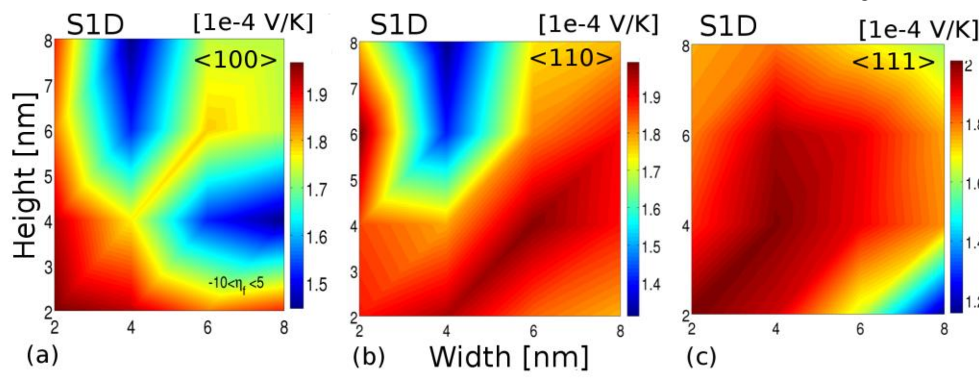


**Fig. 3.** Seebeck coefficient (S1D) at PFmax as a function of W and H for (a) <100> , (b) <110> and (c) <111> oriented wires. <100> wires show symmetric S1D due to symmetric confinement. <110> wires show higher S1D for H confinement compared to the W confinement . <111> wires also show unsymmetrical effect of Y-Z confinement.

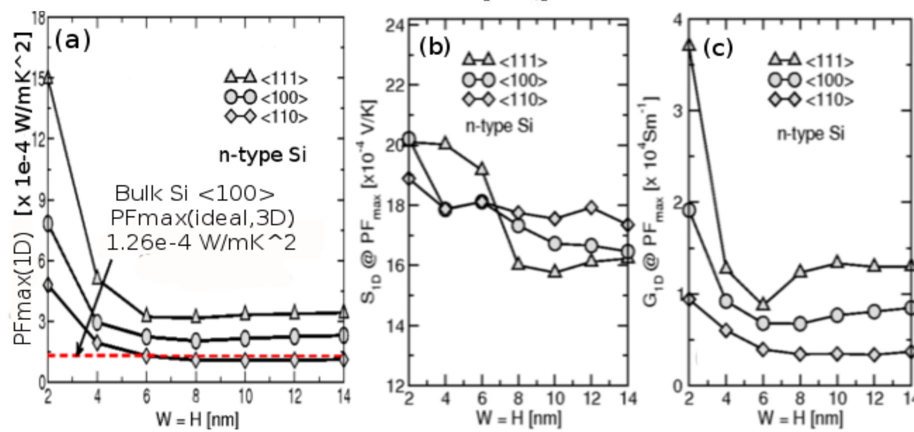


**Fig 4**. (a) Maximum Power-Factor value for <100>, <110> and <111> oriented wires. Significant increase in PF is observed for wires with cross-section dimension (WxH <= 6nmx6nm). <111> shows maximum PF. (b) Seebeck coefficient (S1D) at PFmax. All orientations show very similar values. (c) Electronic Conductance per unit area for three wires. <111> shows the highest value due to maximum valley degeneracy.

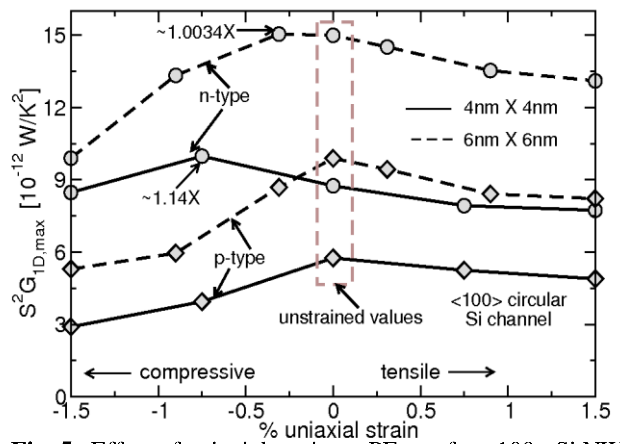


**Fig. 5.** Effect of uniaxial strain on PFmax for <100> Si NW for W/H = 4/4nm and 6/6nm. S1D for n-typecarriers improve for compressive uniaxial strain. For p-type carriers there is no improvement in S1D with uniaxial strain.

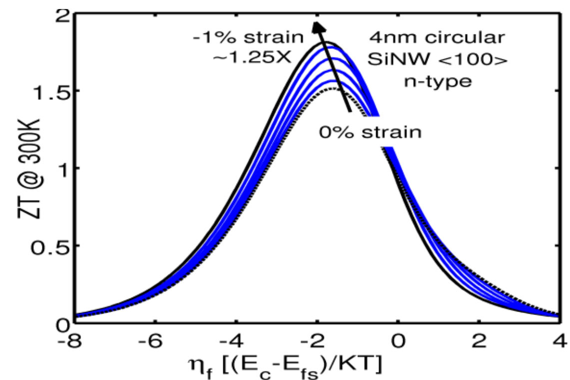


**Fig.6.** Improvement in ZT under compressive uniaxial strain for <100> SiNW for n-type carriers. $\kappa_l$ is taken as 2W/mK as measured for smaller wires. S, G and $\kappa_e$ are calculated using the mode counting method. For 1% compressive strain ~1.25X improvement in ZTmax is obtained compared to the unstrained Si.