Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Strain Engineering of the thermal conductance in Si nanowires

A. PAUL, K. MIAO, M. LUISIER, G. KLIMECK, Purdue University — Silicon nanowires (SiNWs) are promising semiconductor structures spanning a wide range of applications from CMOS devices to thermoelectric modules. Recently, SiNWs have shown tremendous potential as good thermoelectric materials with ZT coefficients larger than 1 [1]. This figure of merit can be further improved by tuning the thermal conductivity of the SiNWs. Here, we show that strain provides a natural way of tuning the thermal conductance of ultra-scaled SiNWs. We utilize a modified Valence Force Field (MVFF) model [2] to calculate the phonon dispersion in these SiNWs under strain and extract their thermal conductance using Landauer's approach. Our investigation shows that uniaxial tensile and hydrostatic compressive help reduce the thermal conductance of SiNWs. For example, a 3nm X 3nm, <100> oriented nanowire undergoing a 2% uniaxial tensile strain exhibits a thermal conductance reduced up to 2.6%, whereas a compressive hydrostatic strain of 2% gives a reduction of around 8%. Thus, strain engineering can prove beneficial in tuning the thermal conductance in Si nanowires and offers an efficient way to further improve the ZT figure of merit. Finanacial support from MSD, SRC, MIND and NSF, computational support from nanoHUB.org under NCN. Refs: [1] A. I. Hochbaum et al., 'Enhanced thermoelectric performance of rough silicon nanowires', Nature 451, no. 7175, pp. 163, 2008. [2] A Paul, M Luisier and G Klimeck, 'Modified valence force field approach for phonon dispersion: from zinc-blende bulk to nanowires.', arXiv:1009.6188v2[cond-mat.mes-hall].

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Date submitted: 27 Nov 2010 Electronic form version 1.4