Thermal Conductivity of Nanowires

Thomas Prevenslik
QED Radiations, Berlin 10777, Germany

Email: thomas@nanoqed.org
Contact: +49 175 506 7507

Abstract: The thermal conductivity of nanowires (NWs) over the last decade has received much attention in heat dissipation of 1-dimensinal nanoscale devices. Analysis methods including Molecular Dynamics (MD) based on phonons are typically used in NW heat transfer. But the NW diameters are submicron and preclude classical MD simulations that assume the atoms have temperature when in fact the Planck law denies atoms in nanoscale structures the heat capacity to conserve heat by an increase in temperature. Indeed, phonons do not even exist at the nanoscale. In contrast, the simple QED method of nanoscale heat transfer based on the Planck law conserves heat in NWs by the emission of EM radiation instead of increases in temperature. Under steady heat flow, EM waves as photons stand across the NW diameter and length that partition the heat in term of dissipation time or inverse of standing wave frequencies. In this paper, the simple QED heat transfer response of silicon NWs is compared with experiment and phonon-based derivations of thermal conductivity of NWs at ambient temperatures from 1 to 300 K.

Keywords: Nanowires, classical physics, Planck law, simple QED, thermal conductivity, ETC

I. INTRODUCTION

One-dimensional 1D NWs have attracted [1] attention over the past decades based on heat transport at the nanoscale by phonons. For silicon NW diameters < 20 nm, the phonon dispersion relation could be modified due to phonon confinement with phonon group velocities significantly less than the bulk value. MD simulations [2] shown 1 nm silicon NWs have thermal conductivities 2 orders of magnitude smaller than that of bulk silicon.

Since then, the transport of thermal energy at the nanoscale is considered [3,4] a ballistic process driven by infrequent collisions between phonons as compared to classical diffusive processes driven by frequent phonon collisions. At the nanoscale, the phonons are more likely to collide with a boundary than with each other making heat transfer by Fourier's law invalid initiating and a search for non-Fourier models of nanoscale heat transfer.

Today, various models have been proposed for nanoscale heat transfer by the ballistic nature of energy transport and size dependence of the effective thermal conductivity (ETC). Currently, variants of the Guyer and Krumhansl [5] model based on phonons is widely used at the nanoscale where the mean free path of the heat carriers is the same order of dimensions of the nanostructure.

II. PURPOSE

The purpose of this paper is to propose the heating of NWs follows the simple QED theory [6] of nanoscale heat transfer based on the heating of silicon NWs. Comparisons are made to experimental data and analytical predictions in the literature.

III. THEORY

Simple QED is a nanoscale heat transfer process based on the Planck law [7] of quantum mechanics differing significantly from that of classical physics. Research in nanoscale heat transfer [8-10] has been reported. But despite advances, there are still challenges in understanding the mechanism of nanoscale thermal transport. Perhaps, researchers have not appreciated the significant difference between classical physics and the Planck law with regard to the heat capacity of the atom illustrated in Fig. 1.

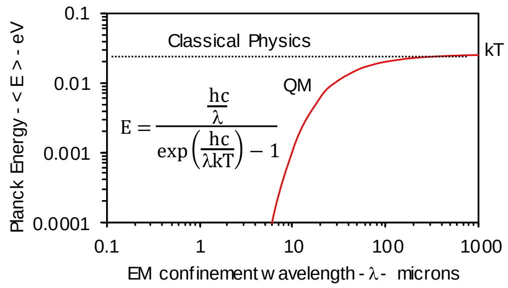

Figure. 1: Planck law of the Atom at 300 °K
In the inset, E is Planck energy, h Planck's constant, c light speed, k Boltzmann's constant, T temperature, and λ the EM wavelength.

The Planck law at 300 K shows classical physics allows the atom constant kT heat capacity over all EM confinement wavelengths λ. QM differs as the heat capacity of the atom decreases for λ < 200 microns, and vanishes at the nanoscale for λ < 100 nm.

Indeed, simple QED by the Planck law denies atoms in nanostructures the heat capacity to change temperature upon the absorption of heat - a difficult notion to accept because of our training in classical physics. QM requires heat transfer to occur without changes in temperature. Here, QED stands for quantum electrodynamics, a complex theory based on *virtual* photons advanced by Feynman [11] and others.

In contrast, simple QED is a far simpler theory that only requires the heat capacity of the atoms in nanostructures to vanish allowing conservation to proceed by the creation of *rea*l photons comprising EM waves that stand within and across the nanostructure.

Similar to electron level quantum states, simple QED quantum states are size dependent based on the dimension of the nanostructure over which the EM waves stand. But brief EM confinement of absorbed heat Q at the surface is necessary to form EM waves standing across and within the nanostructure.

Usually the heating of a nanoparticle (NP) occurs with by an external source of heat having a wavelength $\lambda_o >> d$ that immerses the NP, where d is the diameter of the NP as shown in Fig.2.

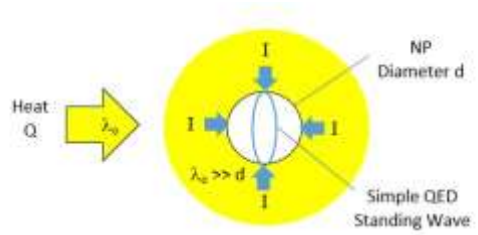

Figure 2. NP heating

The NW differs as Joule heating occurs internally from electrical current and resistance. But again, the heat as IR radiation having $\lambda_o >> d$ effectively immerses the wire cross-section along the wire length similar to the NP. In effect, the NW cross-section is heated by the surrounding heat like the NP from external heating, the inward heat Q flux as a Poynting vector producing the brief EM confinement of the heat Q. But the Planck law precludes conservation of Q by a change in temperature, and instead proceeds by the creation of simple QED radiation in the form of non-thermal standing waves within the geometry of the NW cross-section.

The inward momentum flux I of the Joule heat Q acts as the Poynting vector $S = Q/c$. Taking $U = \pi d^2 S\Delta t$, the momentum flux I of heat Q is, $I = U/c$, where d is the NW diameter and Δt the duration of U. But the momentum flux p of N_p photons standing in the NP is, $p = N_p \cdot h/\lambda$, where λ is the wavelength of simple QED radiation. For $Np \cdot E = \pi d^2 Q\Delta t$, $I = N_p \cdot E/c = N_p \cdot h/\lambda$. Hence, brief EM confinement requires $I > p$, but thereafter Q vanishes and $p > I$ allowing the standing EM radiation to be emitted to the surroundings. Earlier formulations of simple QED based on EM confinement upon the absorption of heat Q in the NP surface is updated here by using the Poynting vector.

The Planck energy E of a photon in the NW cross-section is given by the time τ required for light to travel across and back the NW diameter, $\tau = 2d/(c/n)$, where n is the index of refraction of the NW. Hence, the Planck energy E of the simple QED photons is, $E \sim h/\tau = hc/2nd$ giving the wavelength $\lambda = 2nd$. The simple QED Planck energy E is quantized by the dimension d of the NP that defines the half-wavelength $d = \lambda/2$.

In a NW with different dimensions of diameter d and length L, there are 2 simple QED quantum states. Usually, only the minimum dimension is of importance as by Fermat's principle, the absorbed heat Q is dissipated in the least time. Indeed, most of the heat Q is dissipated across the NW diameter. Taking heat Q as the EM energy in the simple QED standing waves, $Q_d = hc/2nd$ and $Q_L = hc/2nL$.

Importantly, the EM standing waves are non-thermal. The Planck law temperature dependence given by,

$$Q_d = (hc/2nd) \cdot [\exp(hc/2ndkT) - 1]^{-1}$$
$$Q_L = (hc/2nL) \cdot [\exp(hc/2nkT) - 1]^{-1}$$

shows for d <100 nm and T < 300 °K, Q_d and Q_L cannot exist thermally which is precisely why simple QED requires non-thermal EM standing waves. Hence, partitioning of Joule heat in NWs is given by the ratio $Q_L/Qd = d/L$.

IV. APPLICATION

The simple QED application is based on data [1] for silicon NWS having diameters d = 22, 47, 56, and 115 nm with a length L of several microns. The data is about 20 years old and still used today [3,4] to assess consistency with non-Fourier heat transfer models. The bulk modulus of silicon [12] over temperatures from 1 to 1000 °K is shown in Fig.3

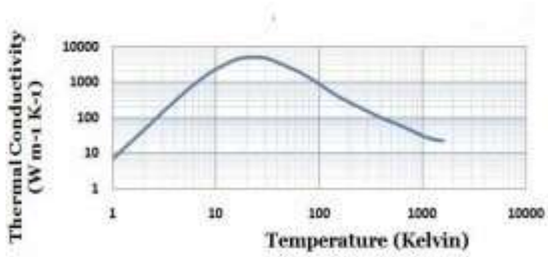

Figure. 3: Thermal conductivity of bulk silicon

In simple QED, the Planck energy E of NW diameters hc/2nd and length hc/2nL depend on the refractive index (RI) of silicon over a wide range of temperatures. Since NW diameters d < 100 nm, the Planck energy E is the EUV to UV which requires RI data at wavelengths < 0.2 microns. Available RI data [13] shows the RI of silicon does not depend on temperature over the full range, but is limited to wavelengths > 0.4 microns. The RI of silicon is given in Fig. 4.

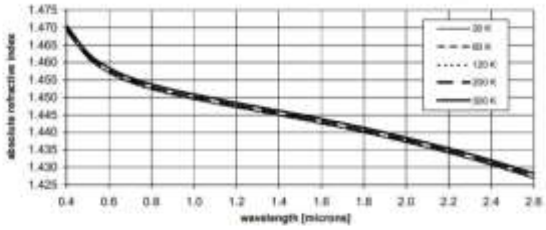

Figure. 4: RI of bulk silicon

Extrapolating the RI data to 0.3 microns gives about n = 1.5 and the simple QED Planck energy E for d = 22, 47, 56, and 115 nm is: 18.8, 8.81, 7.39, and 3.60 eV, respectively. The corresponding wavelengths 2nd are: 66, 141, 168, are 356 nm, all of which in the EUV and UV. Since the NW length [1] is only known to be several microns, the length = 3 microns is assumed giving E = 0.14 eV and 2nL = 9 microns in the FIR.

Simple QED gives the ETC for silicon NWs as the thermal conductivity K of the bulk silicon reduced by the ratio of standing EM waves Q_L/Q_d = d/L. Hence, ETC = K(d/L). The bulk K and reduced ETC on a log-log scale are shown in Fig. 5.

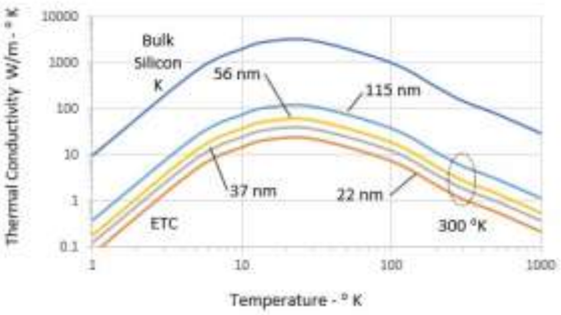

Figure. 5: Bulk K and ETC of silicon NWs

In simple QED, the ETC scale the same with the bulk thermal conductivity K for all temperatures. Over temperatures from 1 to 300 °K, simple QED on a linear-scales is shown in Fig. 6.

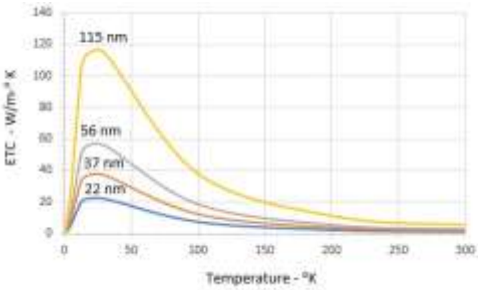

Figure. 6: Simple QED ETC of silicon NWs

Experimental ETC [1] from 30 to 300 °K on a linear scale nare shown in Fig. 7.

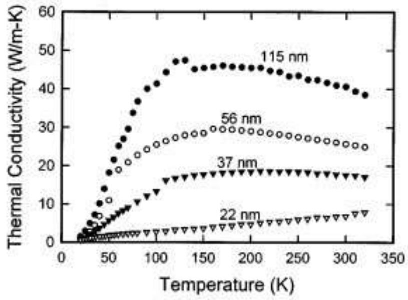

Figure. 7: Experimental ETC of silicon NWs

The ETC are noted in Fig. 5 by an elliptical region at 300 °K. For d = 22 nm, simple QED gives K = 1.1 W/m-°K whereas experiment in Fig. 7 gives K ~ 7 W/m-°K. Even if the NW length L = 2 microns, K = 1.65 W/m-°K, the simple QED prediction is still about 4X lower than experiment.

But the temperature dependence of the ETC in the experiment at temperatures < 300 °K is difficult to understand. Since phonons cannot exist at NW diameters and temperatures, and since the shape of the simple QED prediction of the ETC does not depend on temperature, the only explanation is to repeat the 20 year old experiment to confirm the temperature dependence.

V. CONCLUSIONS

The Planck law denies atoms in silicon NWs the heat capacity to conserve heat by an increase in temperature. Phonons depending on temperature do not exist in NWs. Non-Fourier nanoscale heat transfer models of NWs based on phonons are highly questionable.

Simple QED based on the Planck law conserves heat by the emission of EM radiation. At temperatures < 300 °K, photons instead of phonons carry the heat at the nanoscale consistent with ballistic models

NWs generally thought to reduce heat flow along the wire length are the consequence of most Joule heat being emitted from the wire cross-section as EM radiation into the surroundings. Only a small fraction of Joule heat is loss along the wire length.

ETC has nothing to do with the thermophysical properties of silicon, the bulk and NW silicon properties are the same.

Simple QED applied to < 100 nm NWs shows Planck energies from the UV to the EUV are produced during Joule heat and can be confirmed at the UV level by common UV-VIS spectroscopy.

The significant difference between the shape of ETC curves predicted by simple QED and experiment suggests the experiment should be repeated. Phonon models depending on temperature are not applicable to NWs at temperatures < 300 °K. Only simple QED or other temperature independent ETC models are plausible.

REFERENCES

[1] Li D., et al., 2003. Thermal conductivity of individual silicon nanowires. App. Phys. Lett. 83: 2934- 2936

[2] Volz S. and Chen G. 1999. Molecular dynamics simulation of thermal conductivity of silicon nanowires. Appl. Phys. Lett. 75: 2056 -1999.

[3] Calvo-Schwarzwälder M., et al. 2018. A slip-based model for the size-dependent effective thermal conductivity of nanowires. Intern. Commun. Heat and Mass Transfer. 91:57-63.

[4] Zhang Z., Chen J. 2018. Thermal conductivity of nanowires. Chin. Phys. B, 27: 035101

[5] Guyer R. A., J. A. Krumhansl. 1966. Solution of the Linearized Phonon Boltzmann Equation. Phys. Rev. 148:766.

[6] Prevenslik T. Simple QED Theory and Applications, nanoqed.org, 2015-2020.

[7] Planck M. [1900] On the Theory of the Energy Distribution Law of the Normal Spectrum, Verhandl. Dtsch. Phys. Ges., 2:2-37.

[8] Cahill D. G., et al. "Nanoscale thermal transport," Appl. Phys. vol. 93, pp. 93–818, 2003.

[9] Chen G., Nanoscale energy transport and conversion: parallel treatment of electrons, molecules, phonons, and photons, Oxford University Press, 2005.

[10] Cahill D. G, et al. "Nanoscale thermal transport. II. 2003–2012," Appl. Phys. Rev. vol. 1, pp. 011305, 2014.

[11] Feynman R., QED: The Strange Theory of Light and Matter, Princeton University Press, 1976.

[12] Ziabari A., et al. Adaptive Power Blurring Techniques to Calculate IC Temperature Profile under Large Temperature Variations. See: (PDF) Adaptive Power Blurring Techniques to Calculate IC Temperature Profile under Large Temperature Variations (researchgate.net)

[13] Leviton D., Frey B. D. 2008. Temperature-dependent absolute refractive index measurements of synthetic fused silica - art. no. 62732K.
8 62738Proceedings of SPIE - The International Soc. Optical Eng. 6273