

Nanoscale Heat Transfer by Quantum Mechanics

Thomas Prevenslik

QED Radiations, Discovery Bay, Hong Kong

Abstract

Over the past few decades, the heat transfer of nanoscale structures has been an area of great interest. Classical conduction heat transfer by Fourier theory has been thought unable to explain the reduced thermal conductivity of thin films under Joule heating to justify proposing complex analytical methods based on phonons as ballistic quanta in the Boltzmann transport equation (BTE). However, quantum mechanics (QM) even in its simplest form has been largely ignored. At the nanoscale, QM restricts classical heat transfer by requiring the specific heat of the structures to vanish, a fact that has not been included to date in wide and diverse areas of physics. In this paper, vanishing specific heat is shown to revise our understanding of classical heat transfer because the absorption of electromagnetic (EM) energy in any form cannot be conserved by an increase in temperature. Conservation proceeds by the QED induced up-conversion of the absorbed EM energy to the resonant frequency of the nanostructure and emitted as non-thermal EM radiation. QED stands for quantum electrodynamics. The QED theory is first presented for thin film which is the most extensively studied nanostructure other than nanoparticles (NPs). Other applications of QED heat transfer are discussed including: NP induced DNA damage, nanofluids, nanocatalysts, and the redshift of Galaxy photons in cosmic dust.

Keywords: nanoscale, heat transfer, vanishing specific heat, quantum mechanics.

1. Introduction

Classical heat transfer by Fourier heat conduction theory is generally thought [1-3] not applicable to nanostructures having dimension far smaller than the mean free paths of the electrons and phonons that carry heat to the surroundings. Reduced thermal conductivity is explained by ballistic or non-local heat transfer where the phonons are treated as particles in the BTE.

However, heat transfer by plasmon carriers does not admit [4,5] to rapid transient response, similar to the non-thermal EM emission from NPs under laser irradiations [6] where the photons are not in equilibrium with the far slower phonon rates.

In this paper, QED induced EM radiation is proposed to allow rapid heat transfer in nanostructures by the emission of non-thermal EM radiation. Similarity is found with the QM previously applied [6-7] to NPs where photons are treated as harmonic oscillators through the theory of QED induced EM radiation. Unlike the slow plasmon response in the BTE, QED induced EM radiation allows the structure to promptly respond by EM emission to any gain in EM energy, say by solar and Galaxy photons, lasers, Joule heating, and molecular collisions.

2. Theory

Continuum Fourier theory is generally thought [8-11] to fail as the thickness of thin films become comparable to the mean free path of heat carriers – electrons in metal

and phonons in semiconductors. Therefore, Fourier theory is claimed unable to explain the large reduction in conductivity in the lateral film direction compared to bulk values, thereby justifying the BTE.

However, the effective conductivity only *appears* [12,13] reduced. This is so, because heat gain has been conserved by conductive heat flow alone that excludes EM emission losses, and therefore the effective conductivity *appears* reduced from that of the bulk. In fact, bulk conductivity is not reduced with Fourier theory being valid in thin films.

QED induced EM radiation finds basis in the fact that atoms in thin films are generally under EM confinement that by QM are restricted to vanishing small levels of thermal kT energy. In effect, the heat capacity or specific heat of the film vanish so heat gain cannot be conserved by an increase in temperature. Similar to creating QED photons of wavelength λ by supplying EM energy to a QM box with sides separated by $\lambda/2$, the low frequency Joule energy is induced by QED to be up-converted to the EM confinement frequency of the film, and since the EM confinement is quasi-bound the Joule energy is then conserved by the leaking of the EM radiation to the surroundings.

To illustrate QED induced heat transfer, consider [12,13] a thin film of thickness δ , width W , and length L conserving the absorption of EM energy in the form of Joule heat as illustrated in Fig. 1

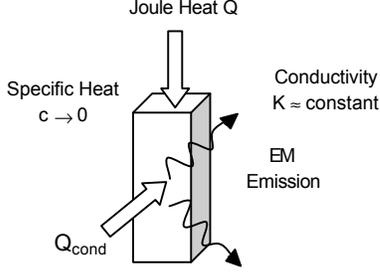


Figure 1. Thin film conserving absorbed EM energy Q by the emission of EM radiation.

2.1. QM Restrictions

QM restricts the allowable kT energy levels of atoms in nanostructures. At 300 K, the Einstein-Hopf relation giving the Planck energy for the harmonic oscillator in terms of kT and wavelength λ is shown in Fig. 2.

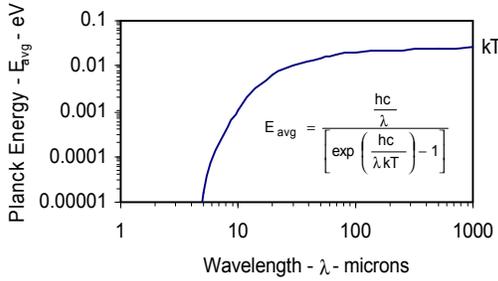


Figure 2. Harmonic Oscillator at 300 K.
In the inset, h is Planck's constant, c is the speed of light, k is Boltzmann's constant, and T is temperature.

For films absent EM confinement, Fig. 2 shows the kT energy saturates for $\lambda > 50$ microns in the far infrared (FIR). Fig. 2 also shows $kT \sim 1 \times 10^{-5}$ eV at EM confinement of $\lambda \sim 5$ microns. Hence, for atoms under EM confinement in nanostructures at $\lambda < 0.020$ microns, the kT energy vanishes.

2.2. EM Confinement

Unlike EM confinement in NPs having the same frequency in all directions, atoms in thin films are only under EM confinement in the thickness direction. For the film as a solid rectangular cavity resonator, the EM confinement wavelength λ is,

$$\frac{1}{\lambda^2} = \frac{1}{(2n_r W)^2} + \frac{1}{(2n_r L)^2} + \frac{1}{(2n_r \delta)^2} \quad (1)$$

For $\delta \ll W$ and L , and $\lambda \rightarrow 2n_r \delta$, where n_r is the solid refractive index. Hence, the film thickness δ defines the EM confinement frequency f , wavelength λ , Planck energy E ,

$$f = \frac{c}{\lambda} \quad \lambda = 2n_r \delta \quad E = \frac{hc}{2n_r \delta} \quad (2)$$

2.3. Vanishing Specific Heat

Classical heat transfer conserves absorbed EM energy by an increase in temperature, but is not applicable to films because of QM restrictions on thermal kT energy. The EM energy U absorbed in the film as Joule heat is induced by QED to create N photons,

$$U = NE = Nhf = N \frac{hc}{2n_r \delta} \quad (3)$$

Since U is non-thermal, the specific heat c_p is,

$$c_p = \frac{\partial U}{\partial T} = 0 \quad (4)$$

Early work by Kelemen [8] recognized that thin films in electronic circuits lacking heat capacity are unstable by themselves under Joule heating. Indeed, the film had to be deposited on a substrate having thickness of a few tens of microns where QM allows the specific heat to be finite to avoid instability.

2.4. QED Induced Transfer

Classical 1-D heat transfer theory in the thickness δ direction is modified by QM for vanishing specific heat and QED induced EM radiation,

$$Q - E \frac{dN}{dt} - K_{\text{bulk}} A \frac{\Delta T}{\delta} = Mc_p \frac{dT}{dt} \sim 0 \quad (5)$$

where, Q is the Joule heat, ΔT is the temperature difference, dN/dt is the rate of QED photons produced having Planck energy E ; K_{bulk} is the bulk conductivity; and $A = WL$ is film area.

Internal film heating given by the product of mass M , specific heat c_p , and temperature rate dT/dt vanishes. Temperature variations in the film are neglected. The Stefan-Boltzmann law for thermal radiation is insignificant at ambient temperature and replaced by QED induced EM emission for non-thermal EM emission. The effective thermal conductivity K_{eff} is upper bound by K_{bulk} ,

$$K_{\text{eff}} = \frac{Q - E(dN/dt)}{A \Delta T / \delta} < K_{\text{bulk}} \quad (6)$$

2.5. Results

Ballistic heat transport in thin films is widely expected [1-3, 8-11] to cause large reductions in thermal conductivity. Typically, the effective conductivity data for thin copper layers at ambient temperature (Fig. 3 of [9]) is reproduced here in Fig. 3. Included is how the EM emission may be inferred from effective conductivity, the respective Planck energy E and rate dN/dt given in Fig. 4.

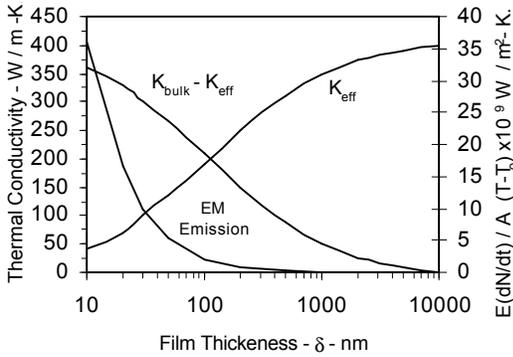


Figure 3. Effective conductivity K_{eff} showing the difference $(K_{bulk} - K_{eff})$ and EM emission $E(dN/dt) / A \Delta T = (K_{bulk} - K_{eff}) / d$

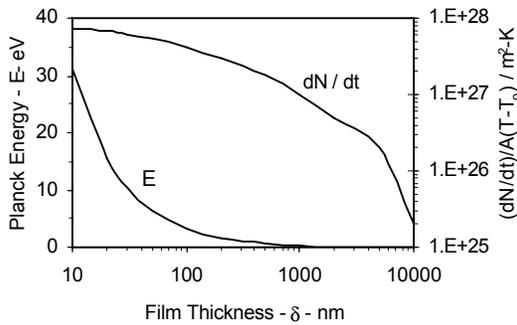


Figure 4. EM Emission Planck Energy E and QED photon rate dN/dt

3. Applications

QED induced heat transfer is used a wide range of diverse applications [14] some of which are presented as follows.

3.1. Nanofluids

Nanofluids comprising NPs in common coolants are found to increase thermal conductivity, but the results to date are questionable because the increases far exceed that given by standard mixing rules.

QED induced heat transfer [7,16] allows the NPs to act as heat sinks to extract heat Q by molecular collisions from the coolant that after QED induced frequency up-conversion to penetrating VUV is absorbed in coolant walls as illustrated in Fig. 5.

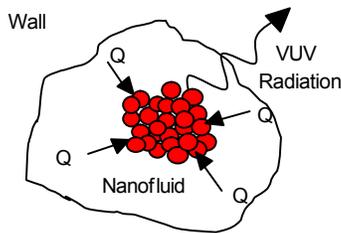


Figure 5. NPs in nanofluid enhancing heat transfer efficiency by non-LTE.

Upon absorption of kT energy from molecular collisions, the NP emits VUV radiation that is not in local thermal equilibrium (LTE) with the FIR radiation absorbed from the collisions. Because of the penetration of the VUV, heat is transferred over greater distances from the NP surface, thereby enhancing heat transfer efficiency. However, the effective conductivity of the nanofluid is not increased above that given by standard mixing rules.

3.2. Nanocatalyst

It is generally thought chemical bonds of reactants are weakened by adsorption to nanocatalysts, but the source of necessary EM energy allowing the reactions to proceed to completion is not well understood. Nanocatalysts are treated [17] as NPs in a solution of reactant molecules A and B in Fig. 6.

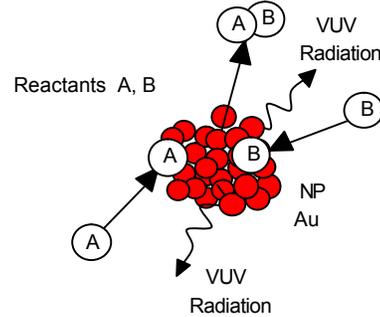


Figure 6. NPs as catalysts in the chemical reaction of A and B to produce AB

Because of EM confinement, the NP atoms have vanishing kT energy, while the free A and B molecules have full kT energy. Collisions transfer full kT energy to the NPs which accumulates and then up-converted to VUV levels by QED, the VUV radiation enhancing the rate by which chemical reactions are completed.

3.3. NP induced DNA Damage

DNA damage induced by NPs is now considered [18] to mimic that by conventional ionizing radiation. UV emission is consistent with the theory of QED induced EM radiation. The NPs need not pass through the cell wall to produce UV radiation upon absorbing the kT energy from colliding water molecules. UV passing through the cell wall is illustrated in Fig. 7.

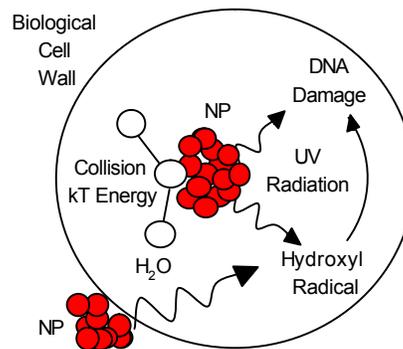


Figure 7. NPs producing UV radiation upon collision of water molecules in body fluids to damage the DNA

QED induced UV radiation from NPs is consistent with experiments over the past decade that have shown NPs < 100 nm produce hydroxyl radicals that cause apoptosis/cell death and single and double strand breaks in the DNA. What enables the NPs to function as an antibacterial agent while posing a health risk is the remarkable fact NPs provide a low level source of continuous UV radiation induced from molecular collisions by QED.

3.4. Redshift of Galaxy Spectral Lines

In 1929, Hubble measured the redshift of galaxy light that based on the Doppler Effect showed the Universe is expanding. However, cosmic dust particles which are submicron NPs permeate space also redshift [14] galaxy light. Fig. 8 depicts a galaxy photon of wavelength λ absorbed in a NP of diameter D and refractive index n_r to create a photon of wavelength $\lambda_o = 2n_r D$. The redshift $Z = (\lambda_o - \lambda)/\lambda$ therefore occurs without an expanding Universe. Hence, dark energy to explain a Universe that is not expanding need not be discovered and allow a return to a static Universe once proposed by Einstein.

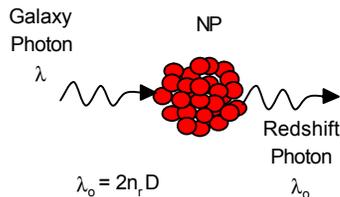


Figure 8. Cosmic dust NP redshift of Galaxy photon

4. CONCLUSIONS

Nanoscale heat transfer by QM that requires the specific heat to vanish is the consequence of not being able to conserve absorbed EM energy of any form by an increase in temperature. Conservation may only proceed by the emission of EM radiation at the confinement frequency of the nanostructure, typically beyond the VUV.

Heat transfer of NPs in biological system by QM shows DNA damage is caused by UV radiation and not by high temperatures.

The EM emission from thin films cannot be predicted by classical methods because finite specific heat allows the Joule heat to be conserved by an increase in temperature. Typically, QM effects become significant only at submicron dimensions.

The BTE analytical method besides being complex is irrelevant because the EM emission from the nanostructure is not included in the heat balance. If included, bulk conductivity is maintained in the film and Fourier heat conduction theory is valid.

Nuclear fuel rod cladding analysis for many years based on finite element programs, e.g., ANSYS represented the thin cladding with bulk properties and clad temperatures coupled to the substrate. Never was the conductivity of the cladding reduced from bulk values.

The fallacy in the BTE method is shown in a thought experiment by irradiating a mirror with a laser and ignoring the light reflected from the surface in the heat balance to determine the mirror thermal conductivity.

Molecular dynamics (MD) analysis [19] did not show bulk conductivity because the atoms were not specified to have zero kT energy in the thickness direction. In a thin film, the only kT energy available is parallel to the surface. MD analysis under zero kT energy in the thickness direction and full kT energy in-plane would have shown no heat flow in the thickness direction and therefore bulk conductivity was not reduced.

The EM emission in the UV and beyond that accompanies the conservation of any form of EM energy in nanostructures can and should be measured with photomultipliers to confirm the correctness of QED induced radiation.

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