Quantum Mechanics Rejects The 30 Year Old Notion Of Reduced Thermal Conductivity In Thin Films

Heat transfer of thin films in electronic circuits is shown to be follow classical Fourier theory using bulk conductivity, although the specific heat is required to vanish.

Feb. 7, 2009 - *PRLog* -- **Background** Classical Fourier theory of heat conduction assumes the bulk conductivity is the same whether the film is thin or thick, and therefore cannot explain the reduced thermal conductivity of thin films found under Joule heating. Over the past 30 years, experiments have shown reduced conductivity for films having a thickness less than about 100 nm. Quantum mechanics (QM) explanations based on the size effect are suggested but none appear in the literature.

Currently, Fourier theory is rejected in the heat transfer analysis of thin films based on the argument the vibration of atoms that transfer heat across the film has wavelengths far larger than the film thickness, the atomic vibrations called phonons. On this basis, Fourier theory has been modified to allow the phonons in the Boltzmann Transport Equation (BTE) to be treated as particles that move across the film thereby overcoming the objection that the thickness of the thin film is far less than the wavelength of the phonons. But the consequence of the BTE is the heat transfer occurs at a lower efficiency that has been interpreted as reduced conductivity.

Typically, the thermal diffusivity "alpha" of a thin film is measured, and this in turn is related to the conductivity K, density "rho", and specific heat c by the relation, alpha = K/ rho*c. One observation is immediately obvious – that the diffusivity alpha diverges as the specific heat c of the thin film vanishes. But why the specific heat c should vanish in a thin film or how this is related to the vanishing conductivity K can not be explained by classical physics.

That the specific heat c vanishes may be inferred from the fact that the conductivity K is currently not measured for the thin film itself, but rather in combination with the substrate. For the film alone, the divergence of diffusivity "alpha" is characterized by erratic measurements over 30 years ago. But with the thin film is attached to the substrate, the diffusivity measurements of the combination are stabilized, although the film conductivity K is found to vanish as the film thickness approaches zero.

Vanishing Specific Heat

The Einstein-Hopf relation provides the QM restriction on the thermal kT energy of an atom as a harmonic oscillator. Here, k is Boltzmann's constant and T is absolute temperature. It important to note the kT energy is electromagnetic (EM). Further, the kT energy rapidly decreases as the EM wavelength vanishes. For films having index of refraction n and thickness d, the EM confinement wavelength w = 2nd, and therefore QM requires the kT energy of films to rapidly vanish as the film thickness decreases. By representing the number N of atoms in the thin film as harmonic oscillators at temperature T, the total energy U (w,T) of the film may be written from which the specific heat c is found by c = dU/dT. Taking the limit on this expression as the wavelength w approaches zero, the specific heat c is shown to vanish.

Atoms in thin films are generally under EM confinement at vacuum ultraviolet (VUV) levels that by QM are restricted to vanishing small thermal kT energy, and therefore the atoms lack the heat capacity to conserve absorbed EM radiation by an increase in temperature. Absent a increase in temperature, the absorbed EM radiation may only be conserved by the emission of EM radiation. At ambient temperature, the boundary between a temperature increase and EM emission is given by the product dn = 5 in units of microns-refractive index. For copper having a refractive index of 2.43, the film thickness threshold for EM emission is about 1 micron.

QED induced EM radiation

Classically, electromagnetic (EM) radiation absorbed in solid bodies is transferred by conduction through atomic vibrations called plasmons, the transfer occurring on the time scale of picoseconds. However, on a far faster timescale, QM allows absorbed EM radiation to also be transferred by photons inside solids only to be emitted as EM radiation. For example, in submicron quantum dots, laser experiments have shown photon emission to occur about 1000 times faster than for phonons, the QED induced emission occurring on the order of femtoseconds.

However, the thermal kT energy of the atoms at ambient temperature is in the far infrared at about 100 microns. Since the films have EM confinement frequencies at VUV levels, and since the lowest frequency allowed in the film is at its EM frequency, the low frequency kT energy is frequency up-converted to VUV levels by QED, the process called QED induced EM radiation. Here, QED stands for quantum electrodynamics.

QM allows one to understand how QED induced EM radiation transfers heat in solids in conjunction with classical Fourier theory. Photons form in all films having the product dn below the threshold boundary. QM requires that any EM radiation absorbed produces photons of a wavelength w depending on the film thickness d, i.e., upon the absorption of EM radiation in a QM box having sides w/2, photons of wavelength w are produced. But only for films having submicron thickness d

Simulation of QM in the Design of Thin Films in Electronics

In the design of thin films in electronics, conductive heat flow in the film parallel to the surface may be neglected. Parallel to the film surface, heat flow essentially occurs in the substrate only, the temperature of the film following the substrate. QED induced EM radiation is emitted normal to the film.

The BTE theory need not be used in the design of electronics circuits. Thermal conductivity K may be assume to remain at bulk values, although the specific heat of the film is required to vanish. In finite element design analysis of film designs, the QM effect may be simulated by selecting zero specific heat for the film in combination with coupling the film and substrate temperatures to each other at the interface.

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About QED induced Em radiation: Classically, thermal EM radiation conserves heat by an increase in temperature. But at the nanoscale, temperature increases are forbidden by quantum mechanics. QED radiation explains how heat is conserved by the emission of nonthermal EM radiation.

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