Simple QED: The Absorption in Raman Scattering?

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Simple QED is a heat transfer process in nanoparticles (NPs) similar to inelastic Raman scattering that changes the frequency of incident light. Interaction of the light with the NP surface occurs as the high surface-to-volume ratio of NPs deposits the heat of absorbed light in the NP surface. But the Planck law precludes temperature increases in NPs, and therefore standing EM radiation is created inside the NP corresponding to a size dependent quantum state having a half-wavelength equal to the dimension over which the EM waves stand.

INTRODUCTION

Classical physics allows the atom to have heat capacity at the nanoscale, the conservation of heat proceeding by a concomitant change in temperature. However, heat transfer at the nanoscale is controlled by the Planck law [1] of quantum mechanics (QM) differing significantly from that of classical physics. Indeed, the Planck law denies the atoms in nanostructures the heat capacity to conserve heat by a change in temperature. Over the past decades, nanotechnology has generally ignored the Planck law and continued to use classical physics to explain nanoscale phenomenon, the consequence of which is an uncountable number of meaningless papers in the literature.

In this regard, 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 prior training in classical physics. Even from personal experience, we know adding heat to an object increases its temperature. But classical physics and our experiences are relevant only to the macroscopic world - not the nanoscale.

Research in nanoscale heat transfer [2-4] has advanced over the past decades, and a large number of interesting phenomena have been reported. But despite the advances in nanotechnology, there are still challenges existing 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 without which nanoscale heat transfer cannot proceed.

Heat transfer without changes in temperature precludes the Fourier law of heat conduction commonly used in nanoscale heat transfer. Similarly, the Stefan-Boltzmann law for radiative heat transfer depending on temperature is not applicable to nanostructures. Although valid at the macroscale, the Fourier law and Stefan-Boltzmann equation are invalid at the nanoscale. Moreover, Molecular Dynamics (MD) simulations [5] based on classical physics thought to provide an understanding of the atomic response to thermal disturbances assume atoms in nanostructures have temperature. An alternative is to formulate nanoscale heat transfer based on the Planck law. In this paper, one such theory called simple QED is presented.

SIMPLE QED METHOD

Simple QED is a method of nanoscale heat transfer analysis that conserves heat with EM radiation instead of temperature. QED stands for quantum electrodynamics, a complex theory based on virtual photons advanced by Feynman [6] and others. In contrast, simple QED is a far simpler theory based on the Planck law that only requires the heat capacity of the atoms in nanostructures to vanish allowing conservation to proceed by the creation of real photons comprising EM waves that stand within and across the nanostructure. Unlike electron level quantum states, simple QED quantum states are size dependent based on the dimension of the nanostructure over which the EM waves stand.

Of relevance to this light-scattering conference, simple QED is similar [7] to Surface Enhanced Raman Spectroscopy (SERS). Unlike elastic Mie theory, SERS is inelastic as excitation laser light is not only scattered from molecules adsorbed to nanostructure surfaces, but also absorbed in both the molecules and the nanostructure as heat, neither of which by the Planck law increase in temperature. Instead, simple QED converts: (a) the heat in molecules to EM radiation at the frequencies of the molecular quantum states, and (b) the heat in the nanostructures is converted to size dependent quantum states of the nanostructure. Typically, the size dependent states are in the EUV and excite lower states by fluorescing down to UV levels to excite plasmon resonances in the IR and VIS.

The Planck law at 300 K is illustrated in Fig. 1(a). By classical physics, the kT heat capacity of the atom is independent of the EM confinement wavelength λ, where k is the Boltzmann constant and T absolute temperature. QM differs as the heat capacity of the atom decreases under EM confinement $\lambda < 200$ microns, and at the nanoscale for $\lambda < 100$ nm, the kT heat capacity may be said to vanish.
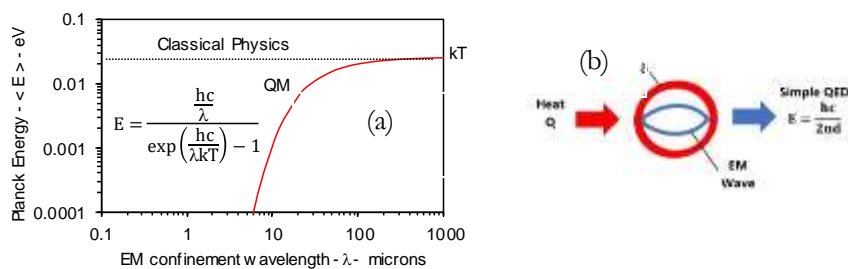

Figure 1. (a) Planck law at 300 K (b) EM heat Q absorption in NP surface

EM confinement occurs by the high surface-to-volume (S/V) ratio of nanostructures that requires laser heat Q to almost totally be confined in the surface, the surface heat itself as EM energy providing the brief geometric confinement necessary to create the size dependent state defined by Planck energy E standing across the nanostructure. Since heat Q is EM energy assumed to have wavelengths greater than the nanostructure dimensions, the heat Q is uniformly distributed over the nanostructure surface. For a spherical NP of diameter d, the heat Q penetrates the surface by thickness δ illustrated in Fig. 1b.

In this regard, the Planck energy E produced in the NP assumes the time τ for light to travel at velocity c/n across and back the NP corrected for the index n of refraction is $\tau = 2d/(c/n)$. Hence, $\lambda = 2nd$ giving $E = hc/2nd$, where h is Planck's constant. For iron at UVC (254 nm), n ~ 1.5. Hence, UVC at 4.88 eV is created in 85 nm NPs.

To confine UVC radiation, the NP boundary requires EM confinement at least equal to the heat Q absorbed in the NP surface. The pressure P acting on the surface is given for a bulk modulus B and volume strain $\Delta V/V$ by, $P = B \cdot \Delta V/V = 6\delta B/d$. But $P = Q/V = 6Q/\pi d^3$ giving $\delta = Q/\pi B d^2$. For 85 nm NPs of iron having $B = 1.6 \times 10^{11}$ Pa, the absorption of a single UVC photon having $Q = E \sim 4.88$ eV gives $\delta \sim 0.2$ fm, a small EM layer, but necessary to geometrically confine the heat Q while creating the UVC photon.

SIMPE QED EXAMPLE

Simple QED is applied to the heat transfer of a spherical iron NP immersed in a liquid bath at constant temperature to illustrate the differences with classical physics as shown in Fig.2.
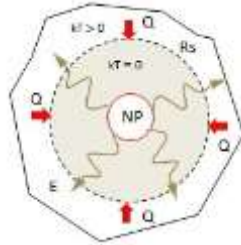

Figure 2. Spherical NP in a Thermal Bath

The NP absorbs heat Q from the thermal bath at absolute temperature T by conduction, while convection is neglected. But Fourier's heat conduction equation is invalid in the bath for kT < 1. The radius Rs at which bath atoms at 300 °K have thermal kT energy is given by the Planck law at EM confinement wavelengths $\lambda \sim 200$ microns shown in Fig. 1(a). For body tissue and water having refractive index n = 1.4, the radius $Rs = \lambda/4n \sim 36$ μm. What this means is the heat flow Q from the liquid at temperature T is converted at Rs to EM radiation in the far IR ($\lambda \sim 200$ μm) and upon being absorbed by the NP is conserved by emitting simple QED radiation. Small temperature changes occur for R < 10 microns, but clearly vanish for NPs < 100 nm.

In classical physics, all atoms in the NP at equilibrium have the same temperature T as the bath. temperature. In terms of the Boltzmann constant k and the number N of atoms, the total thermal energy U is, U = 1.5 NkT. However, by the Planck law the NP atoms do not have kT energy. Instead, simple QED conserves the energy U at equilibrium that otherwise would occupy the NP by creating standing EM radiation inside the NP diameter shown in Fig. 1b. Taking an 85 nm iron NP, the Planck energy E is in the UVC (254 nm), $E \sim 4.88$ eV. The number N of iron atoms is, $N = (\rho V/55) \cdot Av$, where density $\rho = 7854$ kg/m^3, $V = \pi d^3/6 = 3.21 \times 10^{-22}$ m^3, and Av is Avagadro's number $= 6.023 \times 10^{26}$ atoms/kg-mol. Hence, $N \sim 2.7 \times 10^7$ and $U \sim 1$ MeV meaning $\sim 200,000$ UVC photons are created.

The time to create a single UVC photon is estimated [8] assuming 4.88 eV Planck energy E is spread over the spherical surface area πRs^2 of the bath nearest the NP having kT energy. The pulse duration is $\Delta t = 2nd/c = 0.85$ fs. The heat Q required from the bath at Rs to create a

single UVC photon is, $Q = E/\Delta t \sim 900\ \mu W$. For water, $\alpha = K/\rho C = 1.24\ x10^{-7}\ m^2/\ s$ and $K = 0.52\ W\ /m\text{-}K$. Fig.3 shows the temperature drops $\sim 2\ \mu °C$ and recovers in < 1 ps.
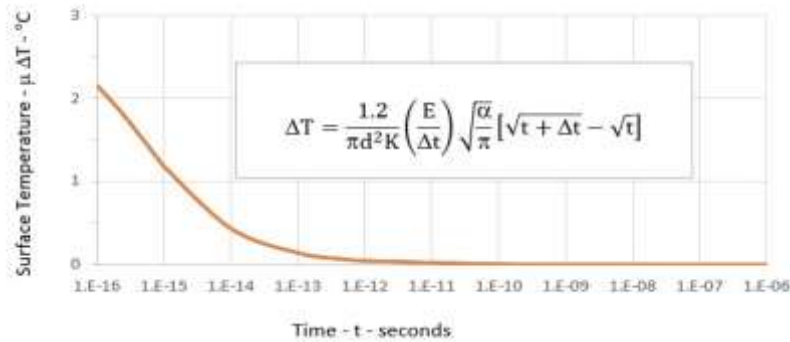

Figure 3. Heat Pulse (900 μW) creating single UVC Photon

CONCLUSIONS

- Simple QED heat transfer in nanostructures is similar to inelastic Raman scattering with absorption allowing the emission frequency to increase or decrease depending on size dependent quantum states defined by the geometry of the nanostructure.
- Application to a single 85 nm iron NP shows the thermal energy equilibrating in a 300 °K bath produces $\sim$ 200,000 UVC photons. Once the UVC photons are emitted, the NP again produces UVC photons and the simple QED process repeats.
- The single UVC photon creation extracts 900 μW from the bath, the bath temperature instantly decreasing an imperceptible $\sim 2\ \mu\ °C$ and recovering in < 1 ps.
- DNA damage by UVC emission from NPs in vaccines accumulating in the brain not repaired by the immune system foretells neuro-degenerative disease and autism.

References
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