



Polymer Nanocomposites by QED Induced EUV Cross-linking

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Nanocomposites comprising NPs in a polymer are observed to display significantly enhanced mechanical properties compared to the polymer alone. NP stands for nanoparticle. The NPs are thought to enhance the polymer properties by forming an interphase, but the mechanism is not well understood. Rationally, the design of nanocomposites cannot proceed without knowing the properties of the interphase. Stress-strain curves are required, but conventional tensile tests are not possible because the interphase is nanoscopic. Currently, MD has been proposed as the method for deriving the properties of the interphase. MD stands for molecular dynamics. But MD simulations based on Lennard-Jones or even ab-initio potentials can never be shown to duplicate the stress-strain curve of the interphase that is unknown. In the alternative, QED is proposed to convert the thermal energy in the NPs during processing to EUV radiation that cross-links the polymer in the interphase to enhance mechanical properties. QED stands for quantum electrodynamics and EUV for extreme ultraviolet. Characterization of the interphase therefore proceeds by obtaining stress-strain curves of macroscopic polymer specimens irradiated at the EUV levels expected during thermal processing of the nanocomposite. Only after MD simulations verify force-fields give the experimental stress-strain data are MD simulations of the NPs and interphase performed.

Keywords: Nanocomposites, Nanoparticles, Interphase, Quantum mechanics, Quantum electrodynamics.

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1. INTRODUCTION

Nanocomposites comprising NPs embedded in a polymer are observed [1] to display significantly enhanced mechanical properties compared to the polymer alone. NP stands for nanoparticle. Enhanced properties are attributed to the interphase comprising a thin < 100 nm polymeric region that forms adjacent the NP surface. Since NPs are typically < 10 nm, the interphase controls the properties of nanocomposites.

Theories [2] of how the interphase explains observed macroscopic properties of the nanocomposites abound the literature, e.g., the models of Lewis, Tsagaropoulos, and Tanaka. All theories assume NPs embedded in a polymer somehow form the nanoscopic interphase adjacent the NPs having properties that explain the macroscopic properties of the nanocomposite. However, no theory identifies the origin of the interphase itself.

Experiments are required to determine the mechanical stress-strain curve of the interphase, but because of its size require nanoscopic tensile specimens, the testing of which is difficult if not impossible to perform. Instead, atomistic MD simulations are generally thought to provide the only way to derive interphase properties. Indeed, MD simulations have been performed of polymer conformation [3] at the NP surface and cross-linking [4, 5] by reactions of chemical radicals.

However, MD is logically fallacious as it is impossible to verify ab-initio estimates of L-J potentials if the stress-strain curve of the interphase is not known. L-J stands for Lennard-Jones. Conversely, if the stress-strain curve of the interphase is known experimentally, MD may be used to adjust the L-J force fields until agreement is found with the experiment. MD could

then be performed for the interphase including the NPs to derive the mechanical response of the nanocomposite. Except for illustrating how the MD simulation would be performed if the L-J force-fields of the interphase were indeed known, the interphase otherwise remains uncharacterized and remains as the nanocomposite dilemma.

How may the nanocomposite dilemma be resolved?

2. CROSS-LINKING MECHANISM

Dilemma resolution first requires a mechanism of enhancement of properties which for polymers can only be cross-linking. Radical polymerization to induce cross-linking may be dismissed as enhancements are observed without photo initiators. UV induced cross-linking requires a source of EM radiation, yet nanocomposites properties are enhanced even if the polymer is known not to exhibit cross-linking. EM stands for electromagnetic. Only if the EM radiation reaches EUV levels do ALL polymers cross-link. EUV stands for extreme ultraviolet. Enhanced properties of nanocomposites are therefore proposed to be the consequence of cross-linking of the polymer by EUV radiation. If so,

What is the source of EUV Radiation?

3. QED INDUCED RADIATION

The source of EUV radiation is the QED induced EM radiation emitted from the NPs as the natural consequence of conserving the absorption of heat from thermal processing the composite under the restrictions of QM. QED stands for quantum electrodynamics and QM for quantum mechanics. The QED emission from a NP is depicted by the green color region in Fig. 1.

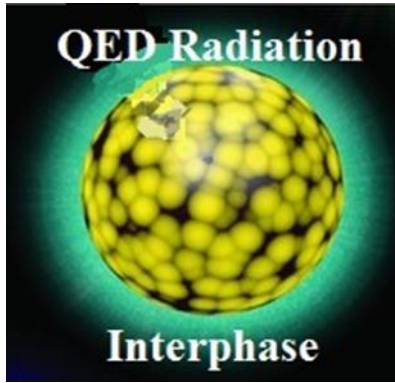


Fig. 1 – QED emission from a NP

The EUV radiation emitted from NPs is not new, having been known [6] for some time as a major source of DNA damage that if not repaired may lead to cancer

3.1 QM Restrictions

QM restrictions on the conservation of heat absorbed in the NPs during thermal processing of the nanocomposite are given by the Einstein-Hopf relation [7] for the harmonic oscillator shown in Fig. 2.

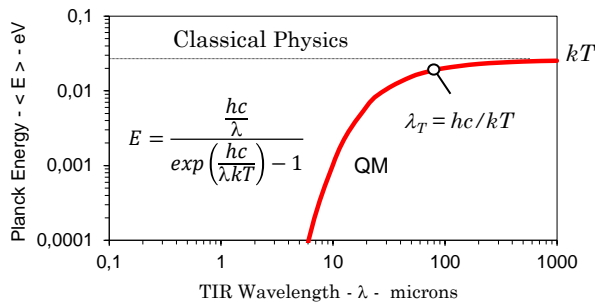


Fig. 2 – The QM restriction of the atom’s kT energy at 300 K. In the insert, E is the average Planck energy of the atom, h is Planck’s constant, c the speed of light, T absolute temperature, and λ the wavelength of TIR confinement. TIR stands for total internal reflection.

Classical physics allows the atom to always have kT energy, but not QM. At 300 K, QM only allows the atom kT energy for $\lambda > \lambda_T = 48$ microns. Conversely, atoms under TIR confinement at wavelengths $\lambda < 6$ microns have significantly reduced $kT < 0.0001$ eV while at the nanoscale for $\lambda < 100$ nm the atom has vanishing heat capacity to conserve absorbed EM energy by an increase in temperature.

3.2 TIR Confinement and QE

Unlike classical physics, QM precludes conservation of heat in NPs by an increase in temperature. Instead, the heat is conserved by the creation of non-thermal EM radiation by QED induced frequency up-conversion to the TIR frequency of the coating.

TIR has a long history. In 1870, Tyndall showed light is trapped by TIR in the surface of a body if its RI is greater than that of the surroundings. RI stands for refractive index. Tyndall used water to show TIR confinement allowed light to be transmitted through

curved tubes. TIR may confine any form of EM energy, although in nanocomposites the confined EM energy is the heat absorbed by the NPs in thermal processing.

TIR confinement requires thermal processing heat to be concentrated in the NP surface that is the consequence of NP absorption having high surface to volume ratios. Therefore, NPs naturally excite the TIR mode of optical confinement. QED under TIR confinement induces the absorbed surface heat to undergo spontaneous conversion to optical surface EM radiation called QED induced radiation. TIR confinement is not permanent, sustaining itself only during the absorption of heat, i.e., absent absorption there is no TIR confinement and QED radiation is not created.

QED relies on complex mathematics as described by Feynman [8] although the underlying physics is simple, i.e., photons of wavelength λ are created by supplying EM energy to a QM box with sides separated by $\lambda/2$. In this way, QED conserves the heat absorbed by the NPs through frequency up-conversion to the optical TIR resonance described by the diameter d the NP. The Planck energy E of the QED radiation,

$$E = h\nu, \nu = \frac{c}{\lambda}, \lambda = 2nd \quad (1)$$

where, ν is frequency and n the RI of the NP.

4. ANALYSIS

The QED radiation emitted from the NPs depends on their RI and diameters d . For zinc oxide and silicon having $n = 2$ and 4, the TIR wavelength given by (1) is shown in Fig. 3.

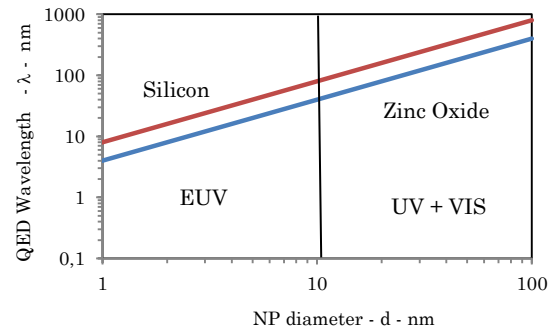


Fig. 3 – QED Wavelength and NP Diameter

The QED emission is in the EUV for $d < 10$ nm and otherwise in the UV and VIS. Optimum EUV enhancement of nanocomposites requires < 10 nm diameter NPs.

5. CHARACTERIZATION

Characterization of the mechanical properties of the interphase is proposed based on uniaxial tensile tests of EUV irradiated polymer using macroscopic tensile specimens in combination with MD or FEA analysis. FEA stands for finite element analysis.

Briefly, characterization proceeds as follows.

1. Prepare polymer tensile specimens, say < 1 mm diameter wires or 3 micron thick flat [9] geometries. The tensile specimens are samples of the natural polymer not yet cross-linked.

2. For the nanocomposite application, determine the wavelength of the EUV emission expected from the NPs based on their diameter and RI using Fig. 3.

3. EUV irradiation of polymers is both complex and very expensive, although table-top [10] sources have recently been developed. Even so, the QED induced EUV source provides a far simpler way of irradiating the tensile specimens as shown in Fig. 4.

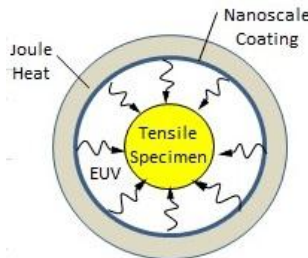


Fig. 4 – EUV Source to Irradiate Tensile Specimens

The EUV source is also based on QED induced radiation, but from a nanoscale coating of say, zinc oxide on the inside surface of a cylindrical vacuum chamber.

In operation, the tensile specimen is positioned axially within a small cylindrical vacuum chamber. Electrical current is passed through the housing by applying voltage in short pulses across the tube length. The electrical current produces Joule heat, but the temperature in the coating does not increase because of QM. Instead, QED conserves the Joule heat by creating EUV radiation that irradiates the tensile specimen. The wavelength of the EUV radiation is given by $\lambda = 2nd$, where n is the RI of the coating and d the coating thickness. For zinc oxide having $n = 2$ and taking $d = 10$ nm, QED creates 40 nm EUV. Other EUV wavelengths require different coating thicknesses, but this is not a problem as a set of cylindrical housings for discrete EUV wavelengths may be provided.

4. Perform tensile tests of the EUV irradiated specimens. Determine the stress-strain curve of the natural and EUV irradiated polymer.

5. For the experimental Young's modulus, derive the elastic stresses adjacent the NP surface using FEA programs, e.g., ANSYS and COMSOL. In FEA, the

RVE is used [11] to derive the nanoscopic properties of the interphase that give the macroscopic response of the nanocomposite. RVE stands for representative volume element. But like MD, the RVE lacks meaning because the Young's modulus of the interphase is not known experimentally.

6. Similarly, perform MD simulations of the EUV irradiated polymer specimen to determine force-fields that give the experimentally derived EUV stress strain before performing MD simulations of the composite comprising both NPs and the interphase.

6. CONCLUSIONS

QED induced radiation based on QM is proposed to provide both a theoretical and experimental basis to the rational design of polymer nanocomposites. The proposal assumes EUV induced cross-linking is available to cross-link all polymers.

7. EXTENSIONS

The QED induced EUV source proposed to irradiate the polymer tensile specimens also allows the extension of Moore's law in the production of computer chips [12] by 13.5 nm lithography as shown in Fig. 5.

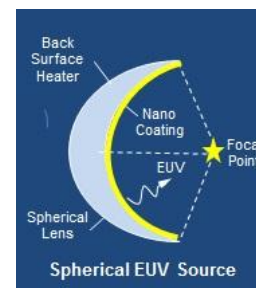


Fig. 5 – QED induced EUV Source in Lithography

In operation, QED induces the heat supplied to the backside of the spherical lens to be converted to EUV using $d \sim 3$ nm zinc oxide coating on the front lens surface thereby allowing 13.5 nm EUV to be focused on the computer chip.

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