Nanocomposites by Quantum Mechanics

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Abstract Nanocomposites with uniform dispersion of NPs offer significantly enhanced mechanical properties. NPs stand for nanoparticles. The composites comprise a large number of NPs in a mold of the desired final composite geometry. The NPs have a metal core encapsulated in a polymer shell. During thermal processing, the shells melt to form a composite that upon solidification form a nearly uniform NP spacing in a polymer matrix, the mechanical properties of which are enhanced as a consequence of QM. QM stands for quantum mechanics. In classical physics, the NP atoms have heat capacity allowing the atoms to increase in temperature during thermal processing. QM differs. By the Planck law, QM precludes the atoms in NPs from having the heat capacity to increase in temperature. Instead, conservation of heat during processing proceeds by QED inducing the NPs to create non-thermal EM radiation that charges the NPs by the photoelectric effect. QED stands for quantum electrodynamcis and EM for electromagnetic. The QED induced EM radiation wavelength is, $\lambda = 2\,nd$, where n and d are the refractive index and diameter of the NP. Coulomb repulsion between the charged NPs produces a triaxial stress state that increases the stiffness of the composite. MD simulations are presented to show that mechanical properties and specifically the Young's modulus of PP are significantly enhanced with a uniform dispersion of NPs. MD stands for molecular dynamics and PP for polypropylene. Absent uniform NP spacing, mechanical properties are not significantly enhanced.

Introduction

Avoiding agglomeration of NPs in a PP matrix is perhaps the central issue [1] in nanocomposites, yet even if avoided; it is unlikely the NP dispersion is uniform. The future of nanocomposites is therefore uncertain unless a process is developed that produces a matrix with a uniform NP dispersion.

In this regard, the process by which a matrix is fabricated with a uniform NP distribution is assumed to be eventually solved by material scientists. In this paper, a process is proposed that may appear difficult to implement, but necessary to proceed with MD simulations that show the Young's modulus of PP is significantly enhanced. The nanocomposite process envisions the production of a large number of preformed NPs placed in a mold of the desired composite geometry as illustrated in Figure 1.

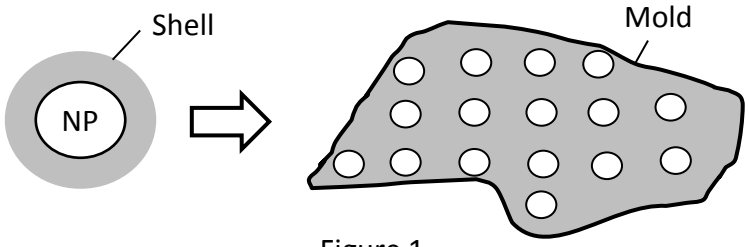

Figure 1
Nanocomposite Thermal Processing

The NPs are assumed to be Fe NPs in a PP shell. A very large quantity of NPs is required. The effort is akin to building a macroscopic object from the bottom–up assembly of atoms. For d = 80 nm Fe NPs in PP shell of thickness t = 210 nm, the NP spacing δ = d + 2t = 500 nm. The NPs are placed in a 3D mold of the desired final configuration as shown in Fig. 1. Thermal processing proceeds by slowly heating the mold to the PP melt temperature, but the mixture is not stirred. Hence, the PP shells melt to form a composite that after cooling forms a nearly uniform spacing of Fe NPs in a solid PP matrix. Experiments are required to determine how well the uniformity of NP spacing is preserved in thermal processing.

Theory

In a PP matrix of uniformly spaced Fe NPs, the mechanical properties are enhanced by the triaxial stress state induced by the Coulomb repulsion of charged NPs, the charging produced [2] as a consequence of QM. External charging is not required. In classical physics, the NP atoms have heat capacity allowing the atoms to increase in temperature during thermal processing. QM differs as shown in Figure 2.

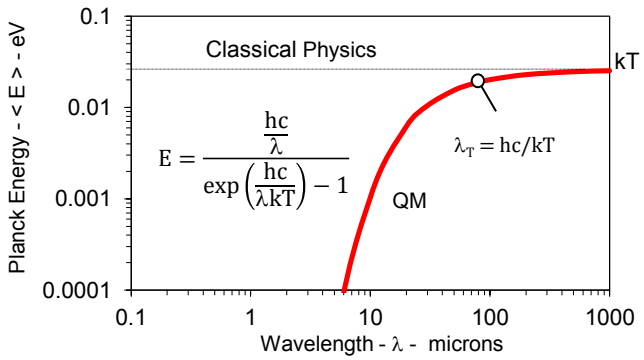

Figure 2. Planck law of the Atom at 300 K
E is Planck energy, h Planck's constant, c speed of light,
k Boltzmann's constant, T temperature, and λ wavelength

By the Planck law at 300 K, QM precludes the atoms at EM confinement wavelengths λ < 100 microns in NPs from having the heat capacity to increase in temperature. EM stands for electromagnetic. In NPs having EM confinement < 100 nm, the heat capacity vanishes, although is significantly reduced at λ < 6 microns.

In thermal processing of NPs, conservation of heat during thermal processing proceeds by QED inducing [3] the NPs to create non-thermal EM radiation that charges the NPs by the photoelectric effect. Metal NPs including Fe are electron-rich and charge positive from ionizing QED radiation produced in the NPs. The QED induced EM radiation wavelength is, λ = 2 nd, where n and d are the refractive index and diameter of the NP. Proper selection of NP properties assures NP ionization during thermal processing. QED induces ionizing EM radiation at 6.21 eV (200 nm) in Fe NPs having n = 1.5, giving the diameter d = 200 nm / 3 $\cong$ 70 nm.

Once the NPs are charged, the polymer should have a low dielectric constant κ to maximize the Coulomb repulsion between other NPs in the matrix, e.g., PP and Teflon have κ = 1.5 and 2, respectively. Moreover, after NP charging, the charge should not decay. In this regard, both PP and Teflon are electret fluoropolymers [4] are claimed to retain charges for a hundred years!

MD Simulation

The MD simulation of the tensile specimen having length L = 10,000 nm and cross-section width W = 2000 nm comprising 500 NPs is shown for a uniform spacing δ = 500 nm in Figure 3.

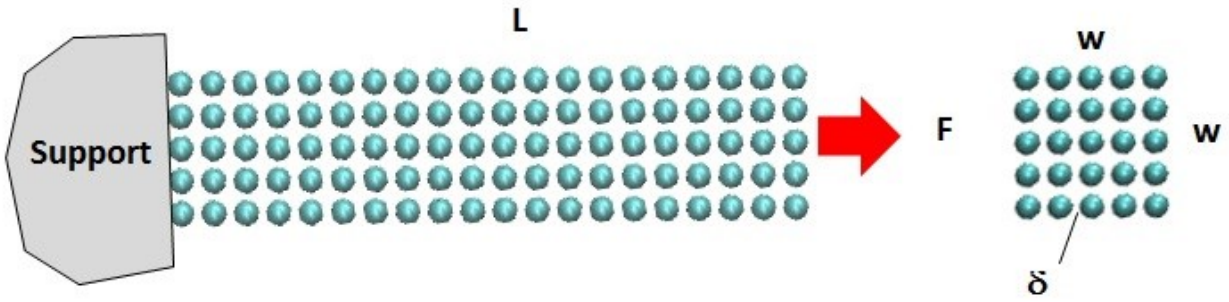

Figure 3
MD Model of only NPs in PP Composite Tensile Specimen

Of importance, the MD model only contains NPs. The PP atoms are not included. To maintain stability under the axial load F, the NPs were free to move in the UZ direction, but were constrained to zero UX and UY displacements in the plane of the cross-section. The UZ displacements at the support were specified to have zero displacement. The force F was imposed by specifying displacement Δ at the free end of the specimen, i.e., $F = (w^2E/L)\,\Delta$, where E is the Young's modulus of PP.

The Coulomb repulsive forces between all NPs alone induce the triaxial stress state that enhances mechanical properties. The Coulomb repulsion is long-range, and therefore all NPs are considered to interact with each other, i.e., no cut-off in force calculations is assumed. The Coulomb force F_c is,

$$F_c = \frac{q^2}{4\pi\varepsilon_o\kappa\delta^2} \qquad (1)$$

where, q is the unit charge, ε_o permittivity, and κ the dielectric constant of PP.

The MD solutions were run at a time step of 5 fs. Convergence to Young's modulus E is rapid in 1000 iterations as shown for spacings 100, 120, 200, 300, and 500 nm in Figure 4. The inset shows simplified estimates the Young's modulus E is inversely proportional to the cube of the spacing between spacings of 100 and 120 nm. At 100 nm spacing, the PP modulus E = $27x10^6$ psi is found. Since the PP modulus = 20,000 psi, the enhancement is about 1000 times. Figure 5 shows at 500 and 1000 nm spacings are shown enhanced about 25 and 2 times, respectively.

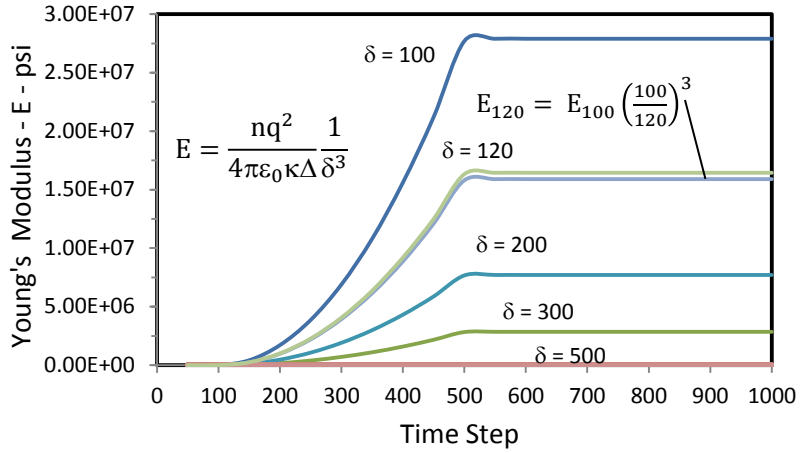

Figure 4
Enhanced Young's Modulus with NP Spacing < 500 nm

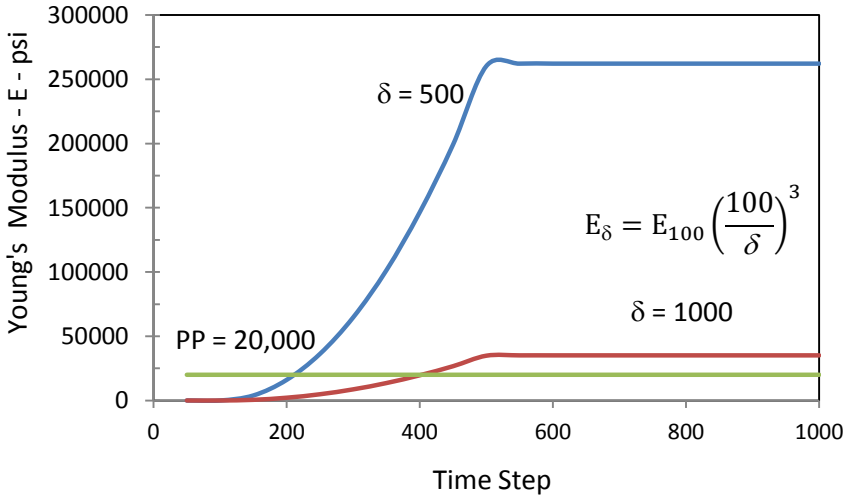

Figure 5
Enhanced PP modulus with NP Spacing < 1000 nm

Discussion

The significant stiffening of PP by uniform NP spacings from 100 to 1000 nm suggests the assumption of lateral constraint by specifying zero UX and UY displacement may be over restrictive. A way of assessing the constraint is to compare the magnitude of the Coulomb force F_c to the lateral displacement Δ of the PP under the lateral F load as shown in Figure 6.

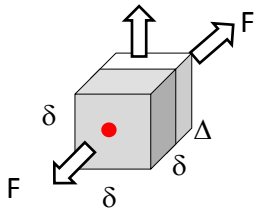

Figure 6

Lateral NP Displacement

The lateral force F is estimated by the Coulomb force Fc between a pair of NPs. For a spacing δ = 500 nm, Equation 1 gives Fc = 6.13×10^{-16} N. The lateral force F exerted on the NP depends on the elastic displacement Δ of the PP, i.e., F = $\delta E \Delta$. For δ = 500 nm and E = 130 MPa, F = 65Δ. As an upper bound, taking F = Fc $\rightarrow$ $\Delta = 9\ 4 \times 10^{-18}$ m << δ = 500 nm. Hence, the PP restrains lateral motion of the NPs making the assumption of zero lateral NP displacements valid.

Conclusions

The MD simulations show triaxial stress state produced by QED induced Coulomb repulsion of charged FE NPs in a PP matrix is significant.

Other forms of charging the Fe NPs should be investigated. Indeed, the electret literature [4] suggests charging under electric fields may suffice. Regardless, the production of electret polymers with submicron uniform NP spacing may be difficult to achieve. Without uniform NP spacing, triaxial stress throughout the extent of the composite cannot be achieved making significant enhancement of mechanical properties unlikely.

References

[1] F. Mirjalili, L. Chuah, and E. Salahi, ‘‘Mechanical and Morphological Properties of Polypropylene/Nano α-Al_2O_3 Composites,” Scientific World Journal, Volume 2014, Article ID 718765.

[2] M. Planck, “On the Theory of the Energy Distribution Law of the Normal Spectrum,” Verhandl. Dtsch. Phys. Ges., 2, 237, 1900.

[3] T. V. Prevenslik, Various QED Applications, See http://www.nanoqed.org , 2010-2016.

[4] B. Gross, *Charge storage in solid dielectrics; a bibliographical review on the electret and related effects*, New York, Elsevier Pub. Co., 1964.