

PREPARATION WITH MODELING AND THEORETICAL PREDICTIONS OF MECHANICAL PROPERTIES OF FUNCTIONALLY GRADED POLYETHYLENE/CLAY NANOCOMPOSITES

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This paper presents preparation with modeling and theoretical predictions of mechanical properties of compatibilized functionally graded and uniform distribution polyethylene/modified montmorillonite nanocomposites manufactured by solution and melt mixing techniques. The morphology is studied by Scanning Electron Microscopy (SEM) and comparisons are made between two techniques. Young's modulus of nanocomposites for functionally graded and uniform distributions is calculated using a genetic algorithm and is then compared with the results of other theoretical prediction models mentioned in the literature as well as experimental results. It is found that the melt mixing technique is the preferred preparation method, and the results obtained from the theoretical predictions of genetic algorithm procedure are in good agreement with the experimental ones.

Keywords: functionally graded material, nanocomposites, solution technique, melt mixing technique, genetic algorithm theory

1. Introduction

Nanocomposites have attracted attention in the recent years because of their improved mechanical, thermal, solvent resistance and fire retardant properties compared to the pure or conventional composite materials. There has been growing interest in polymer/nanoclay nanocomposites in recent years because of their outstanding properties at low loading levels as compared with conventional composites. It has been observed that adding small quantities of nanoclay to some thermoplastics as a reinforcing filler to form nanocomposite materials has not only led to more improved mechanical and thermal properties, but also to enhancement of dielectric strength and partial discharge resistance (Kawasumi *et al.*, 1997; Tan and Yang, 1998; Han *et al.*, 2001; Kornmann *et al.*, 2001; Utracki and Kamal, 2002; Hotta and Paul, 2004; Zhao and He, 2006; Awaji *et al.*, 2009; Chen and Chen, 2009; Kim *et al.*, 2009). As reported in several previous papers (Avila *et al.*, 2008; Nam *et al.*, 2001; Hrachova *et al.*, 2013; Pakdaman *et al.*, 2013; Grigoriadi *et al.*, 2012), some continuum-mechanics based theoretical models have been proposed to predict mechanical properties of polymer/clay nanocomposites. Fornes and Paul (2003) applied the Halpin-Tsai and Mori-Tanaka reinforcement theories to predict the modulus of nylon based nanocomposites. The modulus obtained using Mori-Tanaka calculation increased with nanoclay reinforcement as predicted. The Halpin-Tsai formula gave higher values to the modulus but could still be used to predict its magnitude.

Some efforts have been focused on the modeling of mechanical properties of nanoclay-reinforced polymer composites (Sheng *et al.*, 2004) and nanoparticle-reinforced polymer composites (Smith *et al.*, 2002; Brown *et al.*, 2003). Those modeling efforts have demonstrated the need for the development of a model that would predict mechanical properties of nanoparticle/polyimide composites as a function of nanoparticle size and weight fraction as well as the molecular structure of the nanoparticle/polyimide interface. Although experimental-based research

can ideally be used to determine structure-property relationships of nanostructured composites, experimental synthesis and characterization of nanostructured composites demands making use of sophisticated processing methods and testing equipment, which may result in exorbitant costs. To this end, computational modeling techniques for determination of the mechanical properties of nanocomposites have proven to be very effective (Liu and Chen, 2003; Chen and Liu, 2004; Avila *et al.*, 2006; Haque and Shamsuzzoha, 2003; Isik *et al.*, 2003; Thilly *et al.*, 2009; Dong *et al.*, 2008; Song and Youn, 2006). Genetic algorithms are a family of computational models inspired by evolution. These algorithms encode a potential solution or a specific problem on a simple chromosome-like data structure and apply recombination operators to these structures so as to preserve critical information. Genetic algorithms are often viewed as function optimizers, although the range of problems to which genetic algorithms have been applied is quite broad.

Functionally Graded Materials (FGMs) are inhomogeneous composite materials with gradient compositional variation of the constituents (e.g., metal and ceramic) from one surface of the material to the other, which results in continuously varying material properties. The materials are intentionally designed in such a way that they possess desirable properties for specific applications. Shen (2009, 2011) suggested that the interfacial bonding strength can be improved through the use of a graded distribution of CNTs in the matrix and examined nonlinear bending behavior of simply supported, functionally graded nanocomposite plates reinforced by single walled carbon nanotubes subjected to a transverse uniform or sinusoidal loading in thermal environment. He also investigated post-buckling of nanocomposite cylindrical shells reinforced by SWCNTs subjected to axial compression in thermal environment and showed that the linear functionally graded reinforcements can increase the buckling load. Shen and Xiang (2012) investigated large amplitude vibration behavior of FG-CNTRC cylindrical shells in thermal environments. They assumed that the material properties of CNTRCs were temperature-dependent and solved the equations of motion by an improved perturbation technique to determine nonlinear frequencies of the CNTRC shells.

The present work deals with the preparation and modeling with theoretical predictions of mechanical properties of compatibilized functionally graded and uniform distribution polyethylene/low density polyethylene (LDPE)/modified montmorillonite (MMT) nanocomposites prepared by both solution and melt mixing techniques. The morphology is studied by Scanning Electron Microscopy (SEM) and comparisons are made between the two techniques and then between functionally graded polyethylene/clay nanocomposites with the uniform ones. By using the genetic algorithm procedure, Young's modulus of nanocomposites for functionally graded and uniform distributions is calculated and then is compared with the results of other theoretical predictions models mentioned in the literature and the experimental results. It is found that the melt mixing technique is the preferred method for preparation the functionally graded and uniform distribution polyethylene/clay nanocomposites. Finally, it is shown that the results obtained from the genetic algorithm approach are in good agreement with the experimental ones.

2. Experimental

2.1. Materials

The polymer matrix used in this study was a linear low-density polyethylene with the trade name LL209AA from Arak Petrochemical Co. (Iran), with melt flow index (MFI) of 0.9 g/10 min and density of $\rho = 0.92$ g/cm³. The nanofiller were K10 montmorillonite from Sigma-Aldrich, Germany. Also, the polyethyleneglycol employed in this study was polyethyleneglycol 40 from Merk-KGaA, Germany.

2.2. Processing

2.2.1. Melt mixing technique for uniformed distribution (UD)

An internal mixer from Brabender, Germany (model WHT 55), with roller type rotors and mixer capacity of 55 cm³ was used for preparing nanocomposites samples. The nano clay (MMT) was dried at 40°C in a vacuum oven for a minimum of 48 h. Low density polyethylene (LDPE) and polyethyleneglycol were added to the nanoclay. All materials were manually premixed before introduction into the mixer. The extrusion temperature was set at 140-180°C from the feeder to the die.

2.2.2. Solution technique for uniformed distribution (UD)

The nanoclay (MMT) was dried at 40°C in the vacuum oven for a minimum of 48 h. Low density polyethylene (LDPE) and toluene solution were added to the nanoclay. The mechanical mixture was stirred for 30 min at room temperature. After 30 min of mechanical stirring, the suspension was treated with ultrasound for 20 min. After stirring, the suspension was distilled. The ultrasonic stirring from Hielscher, Germany (model UP400S), was used to ultrasound the suspension.

2.2.3. Melt mixing technique for functionally graded distribution (FGD)

After the melt mixing procedure, the products were then compressed and molded into sheets by an electrically heated hydraulic press. The thickness of every sheet was 1 mm and four sheets with different nanoparticles weight fractions (pure, 1 wt.%, 3 wt.% and 5 wt.%) were employed to form functionally graded nanocomposite. The processing of melt mixing technique for functionally graded distribution is presented in Fig. 1.

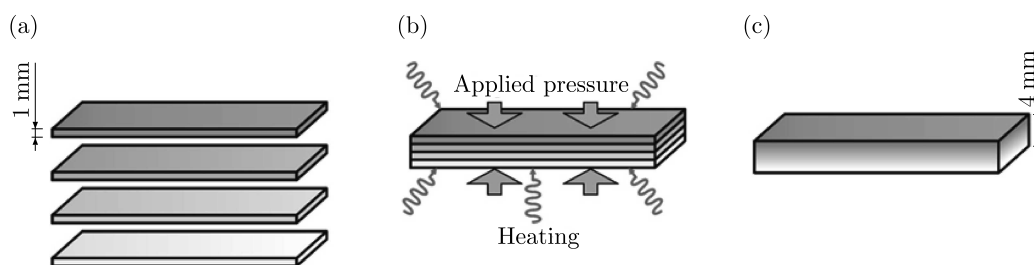


Fig. 1. Processing of melt mixing technique for functionally graded distribution: (a) primary set of nanocomposite sheets with different nanoparticle fractions, (b) processing the FG nanocomposite, (c) fabricated FG nanocomposite

2.3. Scanning electron microscopy (SEM) analysis

The morphology of nanocomposite cross section samples was investigated using a SERON AIS2300C scanning electron microscope. The initial sample preparing process was carried out by a gold-coater chamber. Figure 2a is the SEM photography of the nanocomposite for uniform distribution prepared by the solution technique and Fig. 2b is the SEM image of the nanocomposite for uniform distribution prepared by the melt mixing technique.

Figure 2a shows that the morphology for the solution technique is not homogeneous, which reveals a poor intercalated/exfoliated structure. However, when the melt mixing technique was employed and a compatibilizer was added (Fig. 2b), it was observed that the density and size of the aggregates decreased, which indicated that the dispersion of nanoclays within the polymer matrix was much better. The comparisons between Fig. 2a and Fig. 2b show that the adhesion of the particles of nanoclay and polymer in the presence of the compatibilizer is improved. The

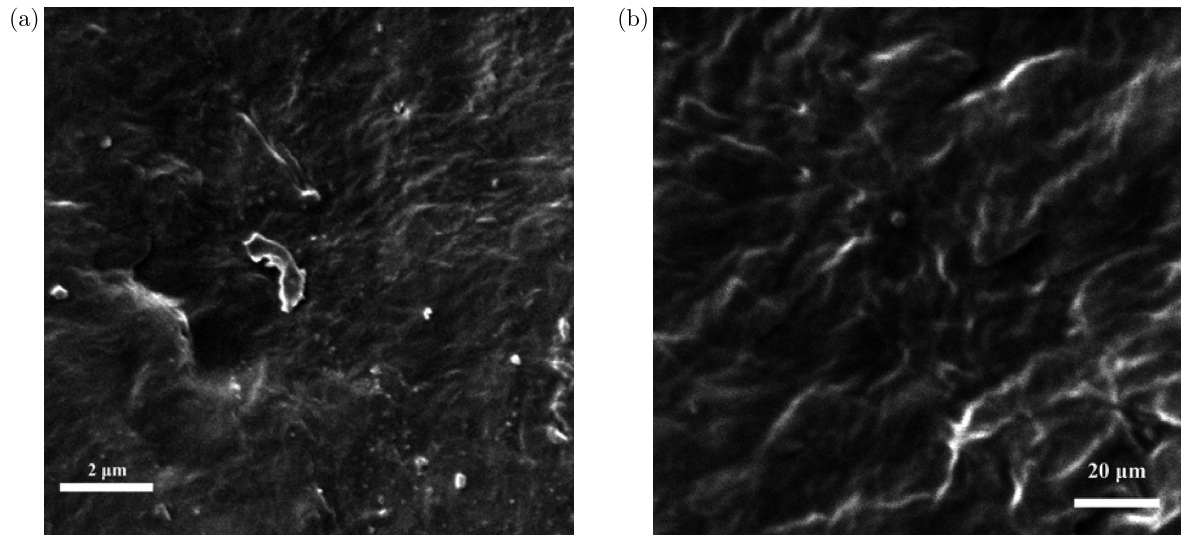


Fig. 2. SEM image of nanocomposite prepared by (a) solution technique and (b) melt mixing technique for uniform distribution

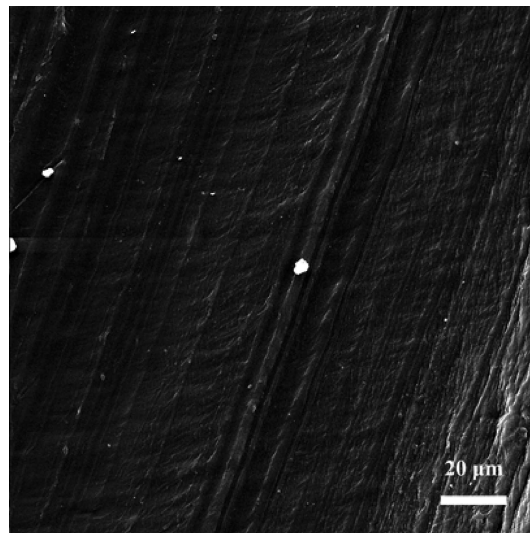


Fig. 3. SEM image of nanocomposite prepared by melt mixing technique for functionally graded distribution

morphology of nanocomposites cross section samples for functionally graded distribution was investigated by a TESCAN MR1A3 SEM after being coated with gold. Figure 3 is the SEM image of the nanocomposite for functionally graded distribution prepared by the melt mixing technique. It seems that the dispersion of nanoclay varies smoothly and continuously from one surface to the other.

2.4. Mechanical properties

The tensile properties were evaluated according to ASTM D638 using dumbbell-shaped samples and a Gotech universal testing machine (Model GT-AI5000L) tensile tester with a crosshead speed of 50 mm/min. The material compositions of the nanocomposites are listed in Table 1.

Figure 4a illustrates the effect of nanoparticles with different weight fractions on the elastic modulus. As noticed, the elastic modulus begins to increase up to 5 wt.% of nanoclay. As the

Table 1. Sample compositions

Sample	LDPE [wt%]	Compatibilizer [wt%]	MMT [wt%]
1	85	15	–
2	82	15	3
3	80	15	5
4	78	15	7

clay weight fraction exceeds 5 wt.%, the elastic modulus levels off, but for functionally graded distribution, the elastic modulus is generally larger than the corresponding values for uniformed distribution of the nanoclay.

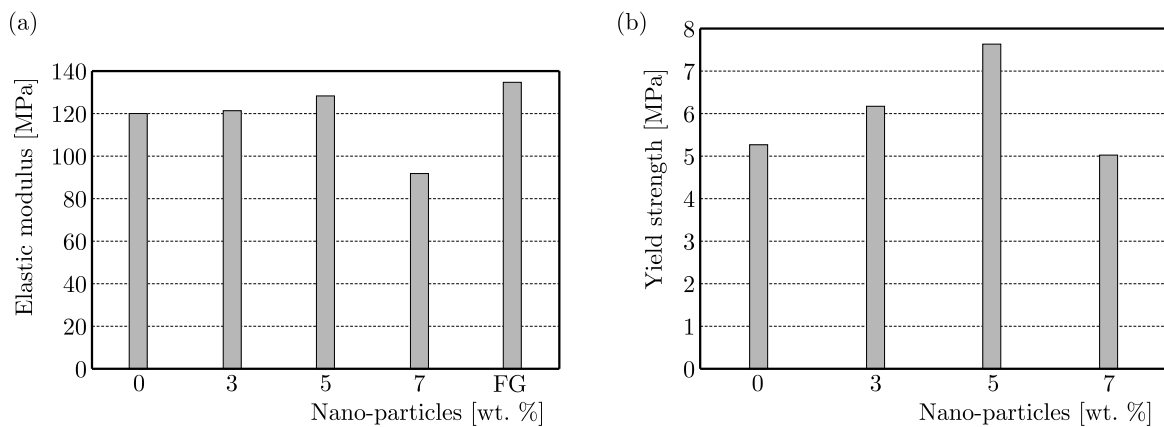


Fig. 4. The effect of nanoparticles with different weight fractions on (a) elastic modulus and (b) yield strength

Figure 4b illustrates the effect of nanoparticles with different weight fractions on yield strengths. As observed, the yield strengths begin to increase up to 5 wt.% of nanoclay. As the weight fraction of clay exceeds 5 wt.%, the yield strengths level off.

3. Modeling

3.1. Theoretical predictions

GA is an unorthodox search or optimization algorithm which was first suggested by John Holland in his book *Adaptation and Artificial Systems* (Holland, 1975). As the name suggests, the GA was inspired by processes observed in natural evolution. The GA method searches for the best alternative (in the sense of a given fitness function) through chromosome evolution. In this paper, the $1 - R_{adj}^2$ is introduced as the fitness function which is to be minimized. R_{adj}^2 is the accuracy criterion of an arbitrary mechanical property function (such as Young's modulus). R_{adj}^2 is defined as a process which is demonstrated below. The mechanical property is a function of nanoclay weight percent and R_{adj}^2 is a function of coefficients which are introduced below. M_i is considered as the mechanical properties and W as the nano clay weight percent. M_1 , M_2 , M_3 and M_4 are Young's modulus, yield stress, ultimate strength and elongation at break, respectively. The M_i is expressed as a polynomial function of W as follows

$$M_i = \sum_{j=0}^4 a_{ji} W^j \quad (3.1)$$

Now, the coefficients a_{ji} are found by maximizing the accuracy of the polynomial function. The equations can be written as:

$$R_{adj}^2 = 1 - \frac{VAR_E}{VAR_T} \quad (3.2)$$

in which

$$\begin{aligned} VAR_E &= \frac{SS_{Err}}{n - k - 1} & VAR_T &= \frac{SS_{Tot}}{n - 1} \\ SS_{Tot} &= \sum_{i=1}^n (y_i - \bar{y})^2 & SS_{Err} &= \sum_{i=1}^n (y_i - M_i)^2 \quad \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \end{aligned} \quad (3.3)$$

and

$$M_i(W) = a_{0i} + a_{1i}W + a_{2i}W^2 + a_{3i}W^3 \quad (3.4)$$

In these equations, $n = 4$ is the number of experiments and $k = 0$ is the number of duplicated experiments and y_i show the experimentally measured mechanical properties. After minimization of $1 - R_{adj}^2$ via MATLAB, the factors a_{ji} are obtained after approximately 40 generations.

3.2. Einstein's model

One of the earliest models developed to predict mechanical properties of composites is Einstein's model (Einstein, 1956)

$$\frac{E_c}{E_m} = 1 + 2.5\phi_f \quad (3.5)$$

where E_c and E_m are the moduli of the composite and matrix, respectively. ϕ_f is the volume fraction of the filler in the matrix.

3.3. Guth and Gold model

The reinforcing effect of spherical colloidal fillers on elastomers was studied by Guth and Gold, and the modulus is given by equation (Guth, 1945)

$$E_c = E_m(1 + 2.5\phi_f + 14.1\phi_f^2) \quad (3.6)$$

where E_c and E_m are the moduli of the composite and matrix, respectively. ϕ_f is the volume fraction of the filler in the matrix. The conversion of weight fractions of nanoclay to volume fractions is shown in Table 2.

Table 2. Conversion of weight fractions of nanoclay to volume fractions

Volume fraction of nanoclay	Weight fraction of nanoclay
3%	1.44%
5%	2.4%
7%	3.36%

3.4. Mori-Tanaka model

A combination of the Mori-Tanaka mean stress concept and the eigenstrain idea of Eshelby's inclusion model was used by Tandon and Weng (1984) to determine the overall elasticity tensor of the nanocomposite materials, assuming that either of the mixture and inclusions (e.g., discontinuous fibers/flakes/nanoparticles) are isotropic or transversely isotropic. For a material reinforced by ellipsoidal particles aligned in the longitudinal direction, the longitudinal modulus may be determined as

$$\frac{E_1}{E_m} = \frac{1}{1 + \frac{1}{A} f_p (A_1 + 2\nu_m A_2)} \quad (3.7)$$

where the subscripts p and m stand for the particles and the matrix, respectively. ν_m is Poisson's ratio of the matrix and f_p are the inclusion particles volume fraction. The constants A and A_i can be calculated from the matrix/particle properties and components of Eshelby's tensor H_{ijkl} (Sheng *et al.*, 2004; Eshelby, 1961; Taya, 1981; Taya and Mura, 1981) which depend on the particle aspect ratio and dimensionless elastic constants of the matrix.

4. Results and discussion

Obtaining the a_{ji} coefficients, Young's modulus can be expressed as a function of the nanoclay weight percent as follows

$$E = -3.401w + 4.97w^2 - 0.677w^3 + 105.338 \quad (4.1)$$

Here, w is the nanoclay weight percent. To investigate correctness of the present results, comparison studies are carried out for Young's modulus of uniform distribution nanocomposites which are presented in Table 3.

Table 3. Comparison of Young's modulus for uniform distribution nanocomposites

Nano clay weight percent	Einstein's predictions [Mpa]	Guth and Gold's predictions [Mpa]	Mori-Tanaka predictions [Mpa]	Theoretical predictions [Mpa]	Experimental results [Mpa]
pure	105.338	105.338	105.338	105.338	105.338
3%	109.130	109.438	126.362	121.586	121.582
5%	111.658	112.513	132.715	127.958	127.939
7%	114.186	115.863	139.412	92.850	92.795

The comparison between theoretical predictions and the experimental data shows high accuracy of the present analysis. Equation (4.1) can be used to derive the suitable relation for Young's modulus of the functionally graded distribution. The specimen with functionally graded distribution consists of four perfectly bonded sheets with a total thickness of 4 mm. Each sheet has 1 mm thickness with different nanoparticles weight fractions (pure, 1 wt.%, 3 wt.% and 5 wt.%). Young's modulus can be written as

$$E(z) = -3.401(2z + \text{sgn}[z]) + 4.97(2z + \text{sgn}[z])^2 - 0.677(2z + \text{sgn}[z])^3 + 105.338 \quad (4.2)$$

As mentioned before, Young's modulus is assumed to vary as a function of the thickness coordinate z ($0 \leq z \leq 4$). Equation (4.2) can be verified via employing static analysis of the functionally graded nanocomposite beam under a transverse load. It is considered as a functionally graded nanocomposite beam as shown in Fig. 5.



Fig. 5. Schematic of the problem studied

The thickness, length, and width of the beam are denoted, respectively, by h , L , and b . The position of neutral surface can be determined as (Yaghoobi and Fereidoon, 2010):

$$h_0 = \frac{\int_{-h/2}^{h/2} E(z)z \, dz}{\int_{-h/2}^{h/2} E(z) \, dz} \quad (4.3)$$

In the Euler-Bernoulli theory, the differential equation of deflection can be expressed as (Yaghoobi and Fereidoon, 2010)

$$\frac{d^2w}{dx^2} = \frac{M(x)}{D} \quad (4.4)$$

where D denotes bending rigidity of the FG nanocomposite beam defined by (Yaghoobi and Fereidoon, 2010)

$$D = \int_{-h/2}^{h/2} bE(z)(z - h_0)^2 \, dz \quad (4.5)$$

Boundary conditions for simply supported and cantilever beams are

$$\begin{aligned} w &= 0 \quad \text{at} \quad x = 0, l \\ w &= 0 \quad \wedge \quad \frac{dw}{dx} = 0 \quad \text{at} \quad x = 0, l \end{aligned} \quad (4.6)$$

By integrating Eq. (4.4) and then applying boundary conditions, Eqs. (4.6), one can easily obtain deflection of the beam under the transverse load. For static analysis of the functionally graded nanocomposite beam under the transverse load, the beam apparatus from TQ, England (Model SM1004), was used for deflection test. The test specimen had a rectangular cross section $(20 \times 4) \text{ mm}^2$ and a length of 15 cm. The load magnitude for both boundary conditions was 0.54 N. The comparison between theoretical and experimental data for the deflection of the functionally graded distribution nanocomposites is shown in Table 4.

Table 4. Comparison between theoretical and experimental data for deflection

Boundary condition	Load position x [cm]	Deflection measuring position x [cm]	Theoretical deflection [mm]	Experimental deflection [mm]
Simply support	5.5	7.5	3.82	3.65
Cantilever	7	15	5.87	5.59

As observed, there is a good agreement between the results. Thus the presented approach for modeling of Young's modulus of functionally graded distribution nanocomposites has high accuracy.

5. Conclusions

This paper presents the preparation with modeling and theoretical predictions of mechanical properties of functionally graded and uniform distribution polyethylene/low density polyethylene (LDPE)/modified montmorillonite (MMT) nanocomposites prepared by both solution and melt mixing techniques. From this study, the following conclusions can be made:

- The mixing technique is generally better than the solution one for preparation of the polyethylene/low density polyethylene (LDPE)/modified montmorillonite (MMT) nanocomposites.
- The compatibilizer plays an important role in improving the properties of polyethylene/low density polyethylene (LDPE)/modified montmorillonite (MMT) nanocomposites.
- By increasing weight fractions of the nanoparticles, the mechanical properties increase up to 5 wt.% nanoclay.
- The elastic modulus for FG distribution of the nanoclay is generally larger than the corresponding value for the uniform distribution of the nanoclay.
- GA is an acceptable optimization research technique which can be used with confidence to identify mechanical properties of nanocomposites with maximum accuracy.

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