STRESS EVALUATION OF NANOCOMPOSITES WITH NANOPLATELETS

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ABSTRACT

Graphite nanoplatelets consisting of one or a few graphene sheets are expected to be an excellent choice for the reinforcement phase of composites. While carbon nanotubes provide reinforcement in just one direction, graphite nanoplatelets are effective in two directions. Thus graphite nanoplatelets will yield a higher degree of stiffening and strengthening in most applications where these reinforcements are expected to be randomly distributed.

In the present paper, a graphite crystal of a layered structure, which is embedded in a polymer matrix, is analyzed to investigate the effect of exfoliation. When the reinforcement volume fraction is kept constant, more uniform layer separation is shown to improve the stiffening efficiency and reduce the stress concentration in the matrix. The analysis result clearly shows the beneficial effect of full exfoliation. The analysis is further extended to the case of random distribution of graphite nanoplatelets with prediction of the resulting composite moduli. The results are discussed with a view toward developing guidelines on the dispersion quality required for the maximum reinforcement efficiency.

KEYWORDS: nanocomposites, exfoliation, nanoplatelets, finite element method

INTRODUCTION

Nanocomposites have lately attracted considerable attention because of the possibility of performance of lightweight, energy-efficient and multifunctional systems. The characteristic of nanocomposites depends on the choice of reinforcement phase and the distribution of reinforcement. As a reinforcement of nanocomposites, Carbon nanotubes have drawn attention due to their high potential to increase the load carrying capability of structural composites [1-4]. While the benefits of continuous nanotubes are obvious, their production still lies far into the future. As a compromise, discontinuous nanotubes could be used to reinforce the matrix. Although being short, on the order of 1 micron or so, these nanotubes are still efficient in reinforcing the matrix due to their high aspect ratio reaching 100 to 1000. According to micromechanical predictions, an aspect ratio of 1000 enables discontinuous fibers to perform almost like continuous fibers as far as the modulus is concerned.

Assuming that the continuum mechanics is applicable, the longitudinal composite modulus E_1 is calculated as follows [5]:

$$\frac{E_1}{E_m} = \frac{1+xW_r}{1-VV_r}, \quad V = \frac{E_r/E_m - 1}{E_r/E_m + x}$$

where, E_r is the Young's Modulus of the reinforcement, E_m is the Young's Modulus of the matrix, V_r is the reinforcement volume content, and x is a parameter depending on the reinforcement geometry. For a fiber of length l and diameter d, the reinforcement parameter is given by

$$x = 2l/d + V_r^{10}$$

For a carbon nanotube, the mechanical properties have not been fully explored. But, the base of the atomic study shows following values reasonable [6].

$$E_r = 1\,\text{TPa}, \; n_{\text{r}} = 0.2$$

where, n_r is the Poisson' s ratio. For a polymer PAN (polyacrylonitrile) used for matrix, the typical mechanical properties are

$$E_m = 3.5\,\text{GPa}, \; n_{\text{m}} = 0.35$$

For carbon nanotubes having a diameter of $d = 1\,\text{nm}$, the aspect ratio can easily reach 1,000 or more and the longitudinal modulus can be as high as above 10 times the matrix modulus for volume content $V_r = 0.04$.

In practice, nanotubes cannot be aligned perfectly in nanocomposites. In the extreme case of two-dimensional random orientation, the composite modulus can be calculated using the laminated theory. Because of the poor stiffening efficiency in the two transverse directions, the quasi-isotropic composite modulus becomes much lower than the longitudinal modulus.

In the case of nanoplatelets that consist of a few graphene sheets, the thickness of a nanoplatelet is on the same order as the diameter of a carbon nanotube. When the nanoplatelet has the same side dimensions as the nanotube's length, its aspect ratio is almost the same as that of the nanotube. Thus the nanoplatelets will yield the same composite modulus in their two planar directions as the longitudinal modulus of a nanotube reinforced composite. That is, the quasi-isotropic modulus of the nanoplatelet composite is the same as the longitudinal modulus of the nanotube composite.

Nanoplatelets are thus ideally suited for reinforcing the matrix phase considering the stiffening efficiency. When graphite nanoplatelets are introduced into fiber-reinforced composites, the resulting composites will exhibit higher stiffness and strength in the transverse directions. In general, nanoplatelets are exfoliated from micron-size graphite crystals and the level of exfoliation directly has an influence on the mechanical properties of nanocomposites. So the study is required to investigate the relation between the level of exfoliation of nanoplatelets and the mechanical properties such as the stiffness and the strength because the distribution of reinforcement is directly determined from the level of exfoliation of nanoplatelets.

In this paper, finite element simulation was carried out to investigate the effect of the level of exfoliation in nanoplatelets on the mechanical properties. Nanocomposites were modeled by a layered structure of graphite nanoplatelets embedded in a matrix. Analysis was carried out for the variation of layer spacing among nanoplatelets with the constant value of the reinforcement volume fraction. Further the analysis model of nanocomposites are extended to a simplified random distribution of graphite nanoplatelets in order to provide the guideline of exfoliation quality required to improve the mechanical properties.

FINITE ELEMENT ANALYSIS OF THE EFFECT OF EXFOLIATION

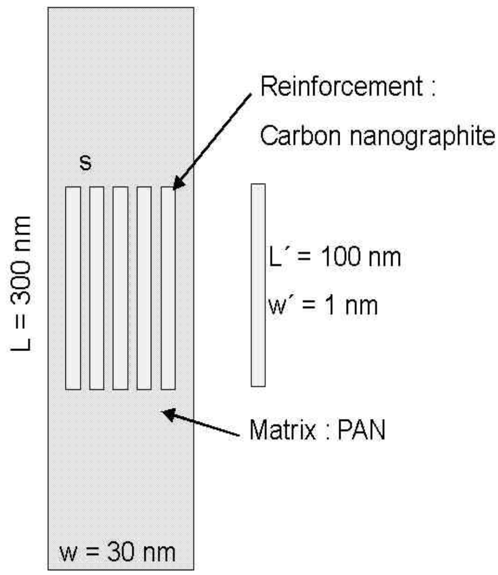
Exfoliation model I : Standard regular distribution of nanoplatelets

The first model of exfoliation is the one in that the nanoplatelet is regularly distributed at the center of matrix. The level of exfoliation depends on the distance between the nanoplatelets. Fig. 1 shows a schematic diagram of the standard regular model for the analysis of nanocomposites. Each nanoplatelet reinforcement has a length $L' = 100$ nm and a width $w' = 1$ nm, thus the aspect ratio reaches to 100 and their volume fraction with respect to the matrix is $1/90$. The material used in the reinforcement is carbon nanographite and the matrix used is PAN (polyacrylonitrile). Table 1 shows the material properties of the reinforcement and the matrix for finite element analysis.

Table1. Material properties of the reinforcement and matrix

Material	Young's Modulus	Poison's ratio
Reinforcement (Carbon nanographite)	1000 GPa	0.2
Matrix (PAN)	3.5 GPa	0.35

Fig. 1 schematic diagram of a nanocomposite exfoliated regularly.



Finite Element analysis of exfoliation model I

Two-dimensional nanocomposites were modeled by a layered structure of carbon graphite nanoplatelets embedded in the PAN matrix. Finite element analysis is was carried out for the variation of the spacing among nanoplatelets from 0 to 4 nm with the constant volume fraction. No spacing between nanoplatelets means that no exfoliation is done. In the present analysis, the interaction between the reinforcement and the matrix is ignored. ABAQUS/Standard, is utilized in order to ensure the accuracy of calculation, a commercial implicit software.

The uniform displacement boundary condition was applied on the one side of nanocomposites while the other side was fixed. The reaction force of nanocomposites and the stress distribution in the matrix are obtained to investigate the effect of the level of exfoliation. Fig. 2 shows the von Mises stress distribution in the matrix at the extension of 10 nm. As increasing the spacing, stress distribution in nanocomposites near the reinforcement becomes uniform and the maximum von Mises stress is decreased. Those results explain that the nanocomposite well exfoliated can support higher load safely. Fig. 3 shows the stiffness of nanocomposites with respect to the level of exfoliation. As the spacing between nanoplatelets increasing, the stiffness of nanocomposites also increases. Two figures show the improvement of the stiffening efficiency in nanocomposites and the reduction of the stress concentration in the matrix proportional to the level of exfoliation. Those results are due to the increase of the portion occupied by the nanoplatelets in the nanocomposites when exfoliation is well performed.

The quantitative comparison of the mechanical efficiency of nanocomposites with respect to the level of exfoliation is shown in Fig. 4. The von Mises stress is decreased more than 20% and the stiffness is increased about 10% while the spacing between nanoplatelets is increased by 4 nm. Analysis results clearly demonstrate that the larger spacing of the layer separation induces the higher performance of nanocomposites in the stiffness and the uniform distribution of stress. The analysis result shows the beneficial effect of full exfoliation.

Fig.2 Distribution of the von Mises stress of nanocomposites with respect to the level of exfoliation

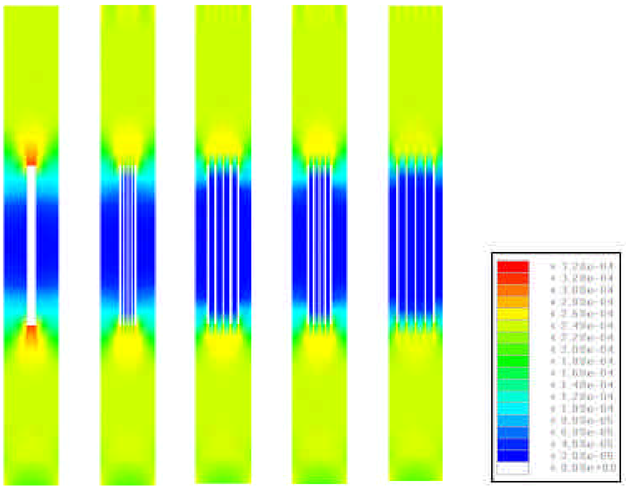


Fig.3 Stiffness of nanocomposites with respect to the level of exfoliation

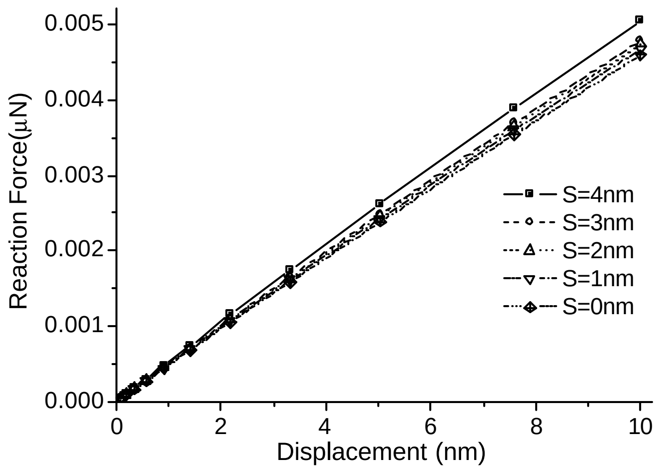
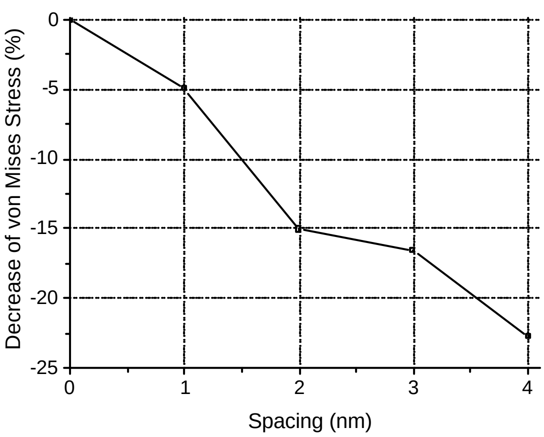
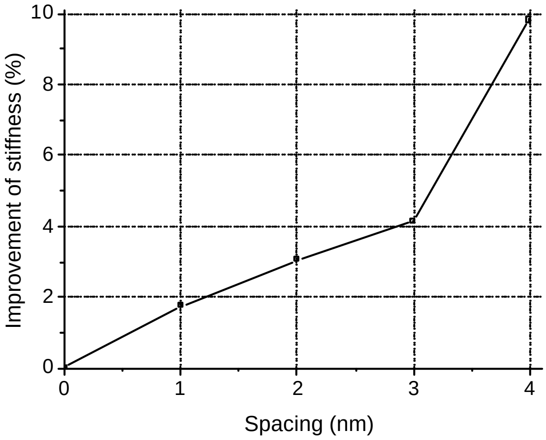


Fig.4 Mechanical efficiency of nanocomposites with respect to the level of exfoliation.

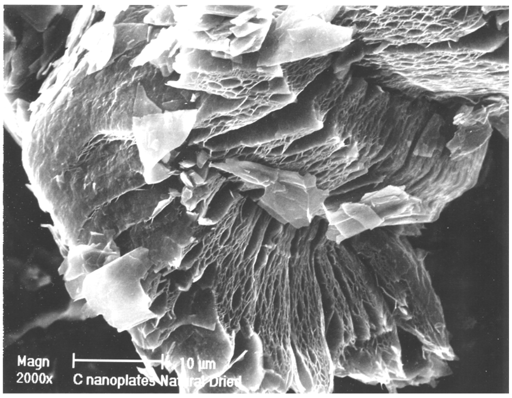




Exfoliation model II: Simplified random distribution of nanoplatelets

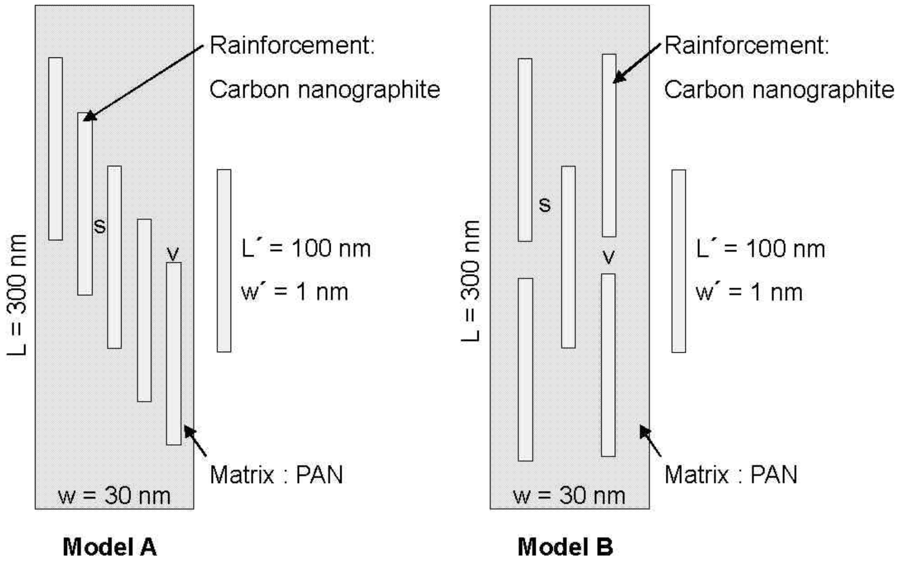
In the previous analysis, nanoplatelets are regularly distributed at the center of matrix. But not all nanoplatelets are expected to be aligned perfectly uniform in practice. In reality, nanoplatelets are randomly exfoliated in the matrix. Fig. 5 shows partially exfoliated graphite nanoplatelets. An analysis model needs to be extended for consideration of the random distribution of nanoplatelets in order to show the effect of exfoliation and to provide the guideline of exfoliation quality required to improve the mechanical properties. But the distribution of nanoplatelets is so random in nanocomposites that it is necessary to simplify the distribution in the model.

Fig. 5. Partially exfoliated graphite pla telets.



In this paper, simplified nanocomposite models are proposed to consider the case of randomly exfoliated nanoplatelets. Fig. 6 shows the two simplified random distribution models. These models may be regarded as a portion of randomly exfoliated nanoplatelets in the matrix. Different nanocomposites randomly exfoliated were modeled by layered structure of carbon graphite nanoplatelets embedded in the PAN matrix. The distribution of nanoplatelets can take variation in two directions. A spacing in the horizontal direction is indicated as a symbol s and in the vertical direction is indicated as a symbol v on both models. Analysis was carried out to show the effect of random exfoliation on the stiffening and stress distribution.

Fig6. Schematic diagrams of simplified random distributed nanocomposites



Finite Element analysis of the random distributed models

Finite element analysis was carried out for the variation of the spacing in the vertical and horizontal direction. Two values in the vertical and horizontal spacing are taken to indicate the level of exfoliation. Analysis models are listed in Table 2. The uniform displacement boundary condition was applied on the one side of nanocomposites while the other side was fixed. The results are compared with the variation of the horizontal spacing and the vertical spacing. The reaction force and the stress distribution in the matrix are obtained to investigate the effect of the level of exfoliation.

Table 2 Variation of spacing in the simplified random distributed model

Model A	Horizontal space (s)	Vertical space (v)	Model B	Horizontal space (s)	Vertical space (v)
A-S1-V20	1 nm	20 nm	B-S1-V20	1 nm	20 nm
A-S3-V20	3 nm	20 nm	B-S3-V20	3 nm	20 nm
A-S1-V40	1 nm	40 nm	B-S1-V50	1 nm	50 nm
A-S3-V40	3 nm	40 nm	B-S3-V50	3 nm	50 nm

In the case of Model A, the von Mises stress distribution in the matrix at the extension of 10 nm is shown in Fig. 7 and Fig.8. The distribution of von Mises stress tends to be uniform as the horizontal spacing is increased in the standard regular model. The tendency is still persists in Model A. But the analysis results of Model A shown in Fig. 7 and Fig. 8 indicate that the distribution of von Mises stress becomes more uniform as the vertical spacing is decreased more. Those results are due to the decrease of the portion occupied by nanoplatelets in the nanocomposites. Fig. 9 and Fig. 10 shows the stiffness of the nanocomposites with respect to the variation of the vertical spacing. Each figure shows the improvement of the stiffening efficiency in nanocomposites with increase of the vertical spacing at a constant horizontal spacing. Figures also indicate that random distribution of nanoplatelets increase the stiffness of nanocomposites. Analysis results fully demonstrate the effect of longitudinal exfoliation of nanoplatelets.

Fig. 7 Distribution of the von Mises stress in Model A with respect to the variation of v at s=1nm.

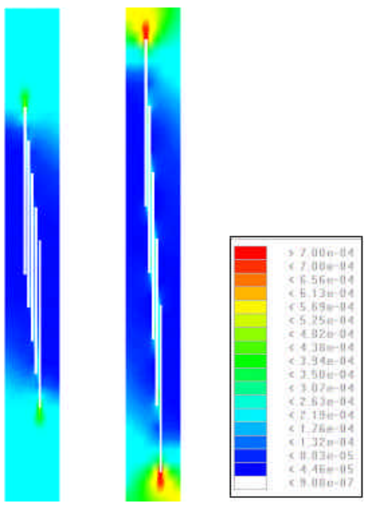


Fig. 8 Distribution of the von Mises stress in Model A with respect to the variation of v at s=3 nm.

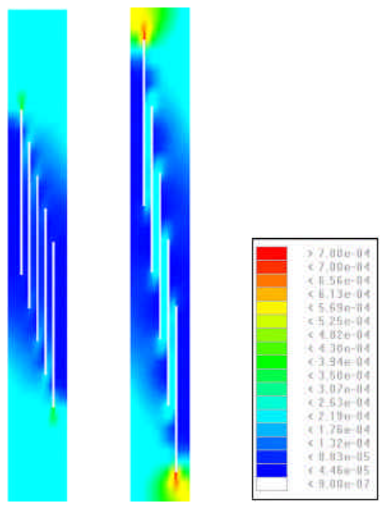


Fig. 9 Stiffness of nanocomposites in Model A with respect to the variation of v at s=1nm.

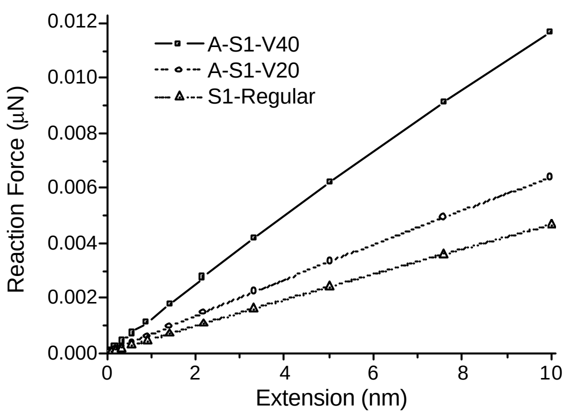
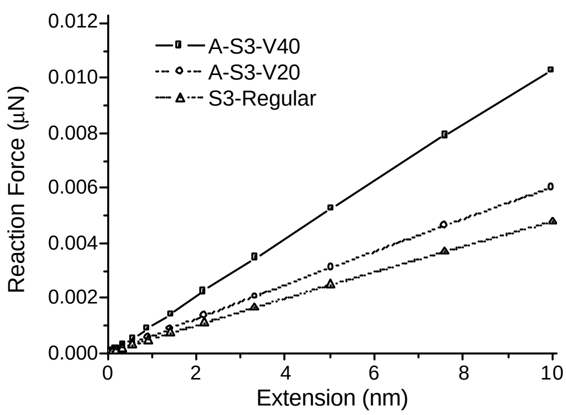


Fig. 10 Stiffness of nanocomposites in Model A with respect to the variation of v at s=3nm.



Nanoplatelets in the simplified Model B are more randomly embedded in the matrix. It can be regarded as a mixed formation of vertical and horizontal exfoliation. The von Mises stress distribution in the matrix at the extension of 10 nm is shown in Fig. 11 and Fig. 12. The reaction force of nanocomposites during the extension is plotted in Fig. 13 and Fig. 14. Comparing with the case of Model A, similar results are obtained for the level of exfoliation in the vertical and horizontal direction. The increase of the vertical spacing in Model B induces the stress concentration in a matrix, but stiffening the nanocomposites. Based on the analysis results, it is possible to estimate the exfoliation quality required for the maximum nanoplatelet' s efficiency.

Fig. 11 Distribution of the von Mises stress in Model B with respect to the variation of v at s=1nm.

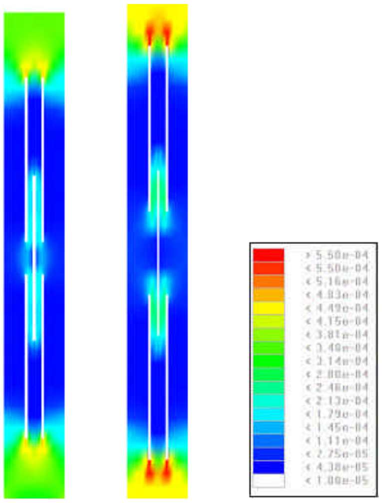


Fig. 12 Distribution of the von Mises stress in Model B with respect to the variation of v at s=3 nm.

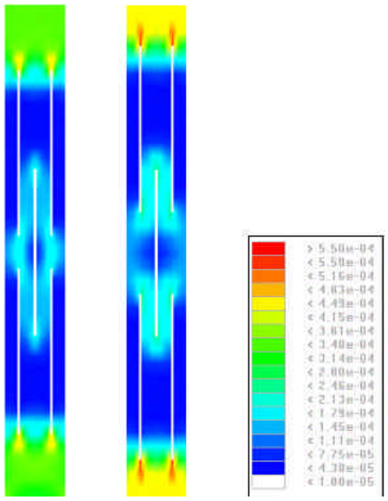


Fig. 13 Stiffness of nanocomposites in Model B with respect to the variation of v at s=1nm.

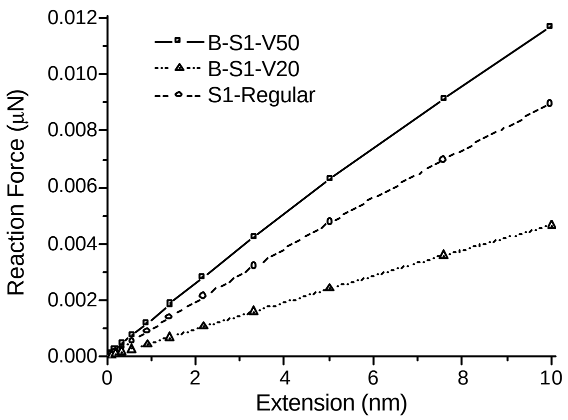
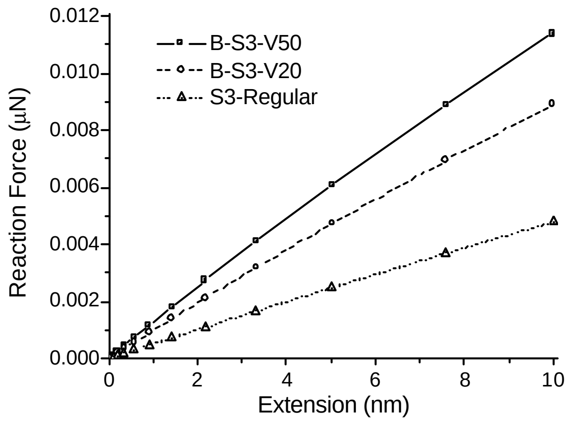


Fig. 14 Stiffness of nanocomposites in Model B with respect to the variation of v at s=3nm.



CONCLUSION

Finite element simulation has been carried out to investigate the effect of the level of exfoliation of nanoplatelets on the mechanical properties. The analysis models represent the model of exfoliation regularly or randomly distributed at the center of the matrix. Analysis results clearly demonstrate the improvement of the stiffening efficiency in nanocomposites and the reduction of the stress concentration in the matrix proportional to the level of exfoliation. Exfoliation models are extended to have random distribution of graphite nanoplatelets. Two simplified models regarded as a part of practice nanocomposites are proposed for the analysis. The vertical and horizontal spacing is considered to denote the level of exfoliation. Analysis results show that the increase of the vertical spacing in Model B induces the stress concentration in a matrix, but stiffening the nanocomposites. These results can be utilized as the guideline of exfoliation quality required to improve the mechanical properties.

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