NUMERICAL MODELS FOR COMPOSITES REINFORCED BY NANO-PARTICLES/FIBERS.

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Abstract

The paper is devoted to description of numerical models that would accurately and efficiently describe behavior of nano-materials and be able to predict its mechanical properties. BIE formulation similar to Method of Fundamental Solutions (MFS) is used but improved and enhanced to fit given purpose. The primary and secondary fields in modeled nano-material were observed with up to 784 of particles/fibers in interaction with each other.

1 Model

In the process of modeling some considerations have to be made. The particles/fibers are considered much stiffer than the matrix and ideal cohesion is supposed between matrix and fiber. The diameter of the fiber is several orders smaller than its length. To accurately model the nano-structure it is necessary to model all kind of effects like fiber-matrix interaction, fiber-fiber interaction and fiber-boundary interaction. The local fields are important for local effect like micro-cracks, and fracturing of the matrix and far fields are important by modeling of larger structures using homogenized replacement of nano-material. The particles are modeled using dipole models where each triple dipole is acting as an autonomous particle. The properties like dimensions and shape can be given by various intensities of the dipole in all three directions. The displacement, stress and strains are computed as follows

$$U_{pi}^{(D)} = \partial U_{pi,p}^{(F)} = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^2}\left[3r_{,i}r_{,p}^2 - r_{,i} + 2(1-\nu)r_{,p}\delta_{ip}\right] \tag{1}$$

$$\begin{aligned} S_{pij}^{(D)} = 2GE_{pij}^{(D)} + \frac{2G\nu}{1-2\nu}\delta_{ij}E_{pkk}^{(D)} = -\frac{1}{8\pi(1-\nu)}\frac{1}{r^3}\Big[(1-2\nu)\left(2\delta_{ip}\delta_{jp} + 3r_{,p}^2\delta_{ij} - \delta_{ij}\right) + \\ +6\nu r_{,p}\left(r_{,i}\delta_{jp} + r_{,j}\delta_{ip}\right) + 3\left(1-5r_{,p}^2\right)r_{,i}r_{,j}\Big] \end{aligned} \tag{2}$$

$$\begin{aligned} E_{pij}^{(D)} = \frac{1}{2}\left(U_{pi,j}^{(D)} + U_{pj,i}^{(D)}\right) = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^3}\Big[-15r_{,i}r_{,j}r_{,p}^2 + 3r_{,i}r_{,j} + \\ +2(1-2\nu)\delta_{ip}\delta_{jp} + 6\nu\left(\delta_{ip}r_{,j}r_{,p} + \delta_{jp}r_{,i}r_{,p}\right) + \delta_{ij}\left(3r_{,p}^2 - 1\right)\Big] \end{aligned} \tag{3}$$

There is strong singularity in stresses and strains.

The fibers are modeled using dipoles which are oriented along the axis of the fiber (Fig. 1). The prescribed boundary conditions are met by solving a system of equations with intensities as unknowns. The fiber is considered rigid and the interactions are based on interacting strains. The method is similar to MFS as it is a meshless method and does not need any integration.

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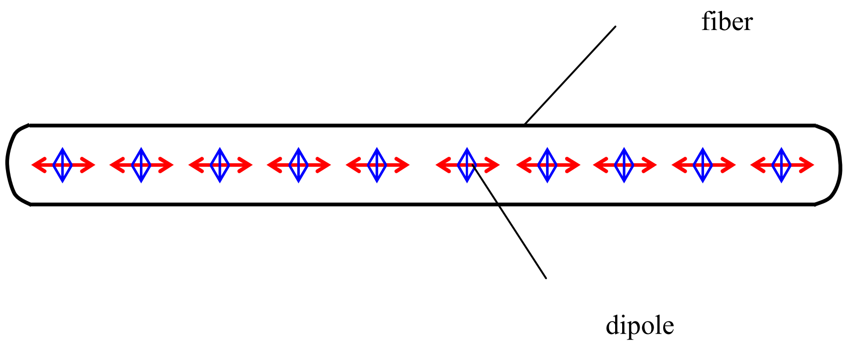


Figure 1: Model of fiber

But if the fibers are very thin a poor accuracy is given as the consequence. Therefore to improve the accuracy polynomial approximation together with continuous source function is used. The integral on the length of the fibers are solved analytically and the approximated by 5[th] order polynomial which gives more simplification to the model and improve the accuracy at the same time. The following integrals have to be evaluated

$$\int_a^b \frac{x_s^n \left(x_s - x_f\right)^p}{\left(y^2 + x_s - x_f^2\right)^{\frac{m}{2}+r}} dx_s = f\left(x_f\right) \tag{4}$$

$$\int_{a+x_f}^{b+x_f} \frac{\left(x + x_f\right)^n x^p}{\left(y^2 + x^2\right)^{\frac{m}{2}+r}} dx = f\left(x_f\right) \tag{5}$$

Intensities of the source functions are smooth along the fiber axis. Minor improvements are needed on the ends of the fiber where the numerical instability causes a fluctuation in the fields.

2 Results

As a result a pack of long fibers have been modeled interacting with matrix and each others. The fiber have aspect ratio of 500, matrix material is linear elastic with young modulus of 1000 and poison number of 0.3. The far field strain is 0.01 and the distance between fibers is 10R in the direction of fiber axis and 3R in the perpendicular direction.

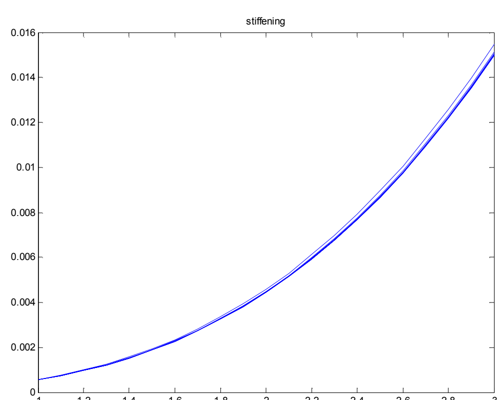
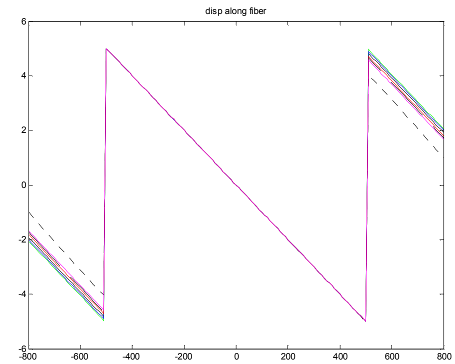


Figure 2: The stiffening effect



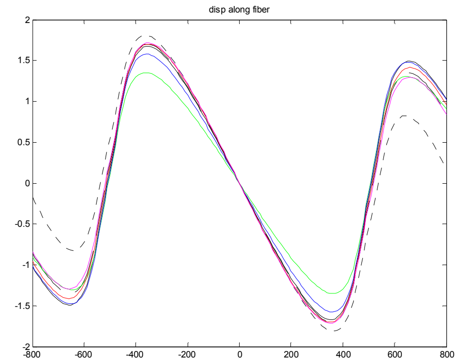
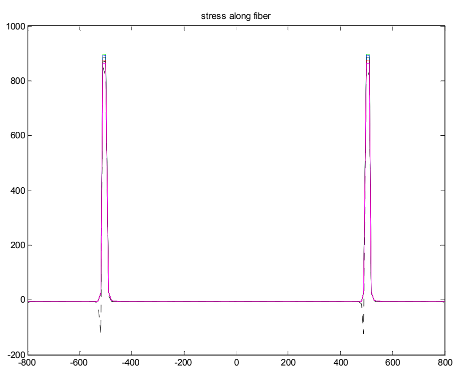


Figure 3: Displacements in the direction of fiber axis on the fiber boundary and in distance 40R from the boundary



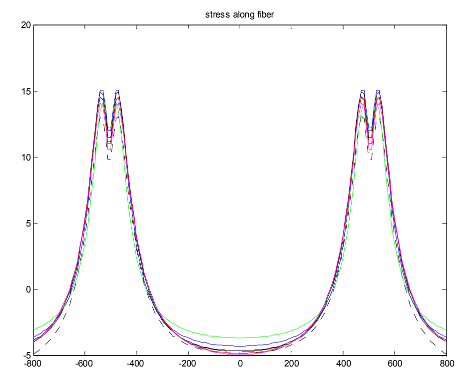


Figure 4: Stresses on the fiber boundary and in distance 40R from the boundary

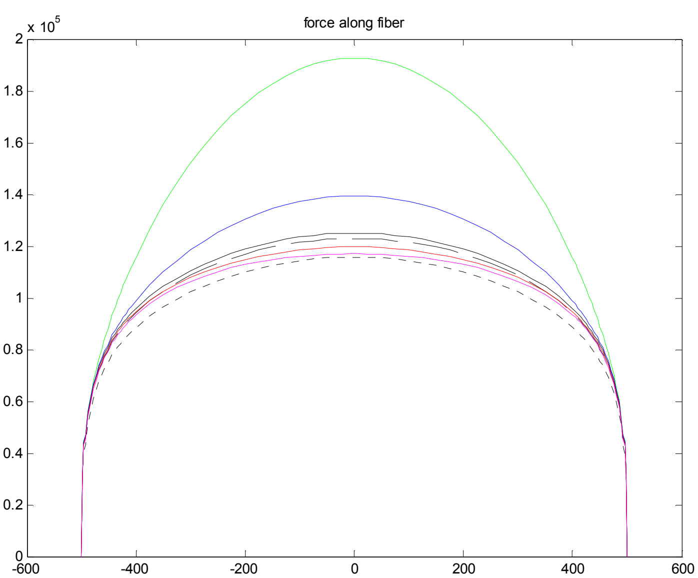


Figure 5: Intensity of the dipoles along the fiber axis

3 Conclusion

In the paper it is shown a method to effective model composite materials reinforced with stiffer particles/fibers. Continuous dipole models enable us to simulate far fields and near fields as well. Due to large gradients worser accuracy is achieved on the ends of the fibers.

References

[1] D. Qian, E. C. Dickey, R. Andrews, T. Rantell. Load Transfer and Deformation Mechanisms in Carbon Nanotube-Polystyrene Composites. *Appl .Physics Letters,* **76:** 2868-2870, 2000.

[2] W. K. Liu, H. S. Park. Bridging Scale Methods for Computational Nanotechnology. In: M. Rieth, W. Schommers, eds. *Handbook of Theoretical and Computational Nanotechnology,* Amer. Sci. Publishers, 2005.

[3] W. K. Liu, S. Jun, D. Qian. Computational Mechanics of Materials. In: M. Rieth, W. Schommers, eds. *Handbook of Theoretical and Computational Nanotechnology,* Amer. Sci. Publishers, 2005.

[4] R. Matsumoto, M. Nakagaki, A. Nakatani, H. Kitagawa. Molecular-Dynamics Simulation of Crack Growth with Crystal Nucleation Amorphous Metal. In: P. Neittaanmäki, T. Rossi, S. Korotov, E. Onate, J. Périaux, D. Knörzer, eds. *European Congress on Computational Methods in Applied Sciences and Engineering,* CD ROM, Jyväskylä, 2004.

[5] Y. J. Liu, X. L. Chen. Continuum Models of Carbon Nanotube-Based Composites Using the Boundary Element Method. *Electronic J. of Bound. Elem.,* **1:** 316-335, 2003.

[6] Y. J. Liu, N. Nishimura, Y. Otani, T. Takahashi, X. L. Chen, H. Munakata. A Fast Boundary Element Method for the Analysis of Fiber-Reinforced Composites Based on a Rigid-Inclusion Model. *ASME Journal of Applied Mechanics,* **72:** 115-128, 2005.

[7] V. I. Blokh. *Theory of Elasticity,* (in Russian), University Press, Kharkov, 1964