Modelling of composites reinforced by micro/nanoparticles using dipoles

MÁRIO ŠTIAVNICKÝ[1]*, VLADIMÍR KOMPIŠ[1], MICHAL KAUKIČ[2]

Composite materials reinforced by stiff particles possess higher stiffness, strength, better wear resistance and superior thermal and electrical properties. Special models are presented based on singular and hyper-singular source functions for modelling composites reinforced with micro/nanoparticles. In global, the model of each particle is represented with triple dipole which is describing the interaction effect of the rigid particle with the matrix. The intensities of the dipole are evaluated on detailed model from boundary conditions. The displacement, stress and strain fields are described by combination of Kelvin's solution and dipole functions acting in infinite domain with singularity outside the domain. The governing equation is automatically satisfied by these functions so it is only necessary to fulfil the boundary conditions. Using such functions, also problems can be solved in which the stiffness of the particles is much higher than the stiffness of the matrix and its one or two dimensions are much smaller than the others, i.e. in the situations when the FEM and BEM models do not work well.

K e y w o r d s: composite, nanoparticle, Method of Fundamental Solutions (MFS), dipole functions, meshless method

1. Introduction

The nanomaterials reinforced by nanoparticles are excellent type of materials with superior mechanical properties [1, 2]. Special properties of surface and volume can be produced by changing the shape or material of nanoparticles and the material of the matrix. It is known that only 1 % of particles might increase the stiffness of the resulting material by 40 % and gives the material special surface qualities like wear resistance. It is therefore necessary to develop numerical procedures that can overlap these countless many options in nanomaterials and model its behaviour

[1] Department of Mechanical Engineering, Academy of the Armed Forces of Gen. M. R. Štefánik, 031 01 Liptovský Mikuláš, Slovak Republic

[2] Faculty of Management Science and Informatics, University of Žilina, Veľký Diel, 010 24 Žilina, Slovak Republic

* Corresponding author, e-mail address: stiavnicky@aoslm.sk

under different circumstances. As it is true that in small volume might be up to few billions of small particles, it would be imperial to produce numerical methods with great efficiency in handling large amounts of particles. Omitting special methods like fast multipole method [3], this is what classical methods like FEM and BEM are lacking of [4–6]. In between any methods which require numerical tessellation became extremely ineffective with large amount of multiscale volumes. Indeed this is the case for nanomaterials with its billions of small nanoparticles enclosed in a large area compared to size of these particles. The main idea in handling multiscale models is not to use any discretization at all.

There are number of meshless methods which could be used for easy manipulation of nanomaterials. Using special type of functions called Trefftz functions [7–9] which apriori fulfil the governing equations puts these methods in advantage over competition. Also fundamental solutions are a kind of Trefftz functions. A method is presented here which has evolved from the Method of Fundamental Solutions or MFS [10–13]. In the method of MFS none of the volumes are discretized, only the boundaries are appropriately covered by field points in which it is necessary to fulfil the boundary conditions. The points can be chosen randomly on any surface, where are boundary conditions to be satisfied. Then it is necessary to choose source points outside the domain of interest where the point forces are going to act. By linear combination of the intensities of the forces acting in source points it is possible to fulfil all boundary conditions. The problems could occur if the distance of the source points measured from boundaries is small compared to the distance between the source points because the source functions will be unable to catch the large gradients between the field points and as a result degraded accuracy might occur. On the other hand when the source points are located far from the boundaries compared to the distance between them, a badly conditioned system

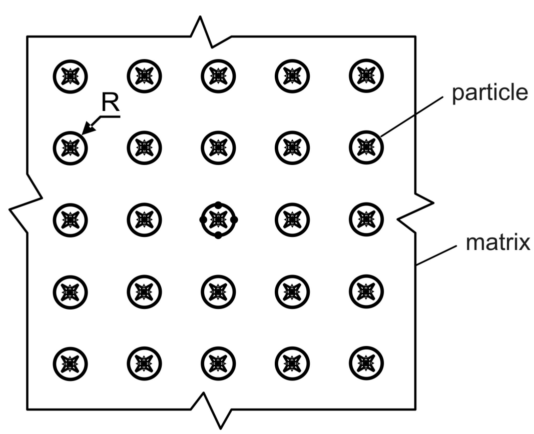

Fig. 1. Matrix reinforced by uniformly distributed particles with dipoles depicted. The particle of interest with collocation points on the boundary is located in the centre.

of equations might occur. Also it could be evaluated that for good accuracy there is needed large number of both source and field points along the boundaries. In problems with complicated surfaces this becomes less and less efficient. Composites reinforced with nanoparticles represent a problem in which a large number of particles are present which can be of the same shape (Fig. 1) and thus a different approach of modelling is more suitable.

In order to calculate the response of real material, a patch containing a given amount of particles is considered. Increasing the number of the particles and accordingly the size of the patch up to the point that the change in the response is negligible, a patch with desired dimensions is retrieved where all particles beyond this patch in a real material would have negligible influence on its response, and so a large reduction of the problem can be done.

2. Method of source functions

In this paper the field caused by every particle in the composite material is described by triple dipole located in the centre of particle. Note that this is only accurate for particles that are of spherical shape, ellipsoidal, or smooth regular surface, as it is supposed to be in this paper.

The displacement field in the direction i of a dipole (two collinear point forces with opposite orientation) acting in direction p can be obtained from the displacement field of a unit force acting in infinite homogeneous domain (Kelvin's solution) by differentiating it in the direction of the acting force [14–17], i.e.

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

where G and ν are shear modulus and Poisson's ratio of the material of the matrix, δ_{ip} is the Kronecker's delta and r is the distance between the source point s where the dipole is acting and a field point t, where the displacement is introduced, i.e.

$$r = \sqrt{r_i r_i}, \qquad r_i = x_i(t) - x_i(s). \qquad (2)$$

With summation convention over repeated indices,

$$r_{,i} = \partial r / \partial x_i(t) = r_i / r \qquad (3)$$

are the directional derivatives of r.

Gradients of displacement field are

$$U_{pi,j}^{(D)} = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^3}\left[-15r_{,i}r_{,j}r_{,p}^2 + 3r_{,i}r_{,j} \right. \\ \left. + 2(1-2\nu)\delta_{ip}(\delta_{jp} - 3r_{,j}r_{,p)} + 6r_{,i}r_{,p}\delta_{jp} + \delta_{ij}(3r_{,p}^2 - 1)\right] \tag{4}$$

and corresponding strain and stress fields are

$$E_{pij}^{(D)} = \frac{1}{2}\left(U_{pi,j}^{(D)} + U_{pj,i}^{(D)}\right) = -\frac{1}{16\pi G(1-\nu)}\frac{1}{r^3}\left[-15r_{,i}r_{,j}r_{,p}^2 + 3r_{,i}r_{,j} \right. \\ + 2(1-2\nu)\delta_{ip}\delta_{jp} + 6\nu\left(\delta_{ip}r_{,j}r_{,p} + \delta_{jp}r_{,i}r_{,p}\right) \\ \left. + \delta_{ij}(3r_{,p}^2 - 1)\right], \tag{5}$$

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

The summation convention does not act over the repeated indices p here.

The fields defined by a dipole have strong singularity in displacements and hyper-singularity in strain and stress fields. Displacement and stress in the direction z of circular area by a dipole located at its centre are depicted in Figs. 2 and 3, respectively.

The stiffening effect of the particles in the matrix is computed from the patch as a ratio of composite stiffness related to matrix stiffness (Fig. 4):

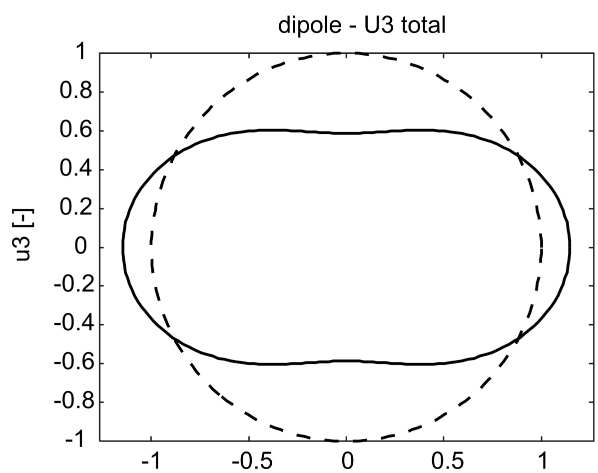

Fig. 2. Displacement of circular area by a dipole.

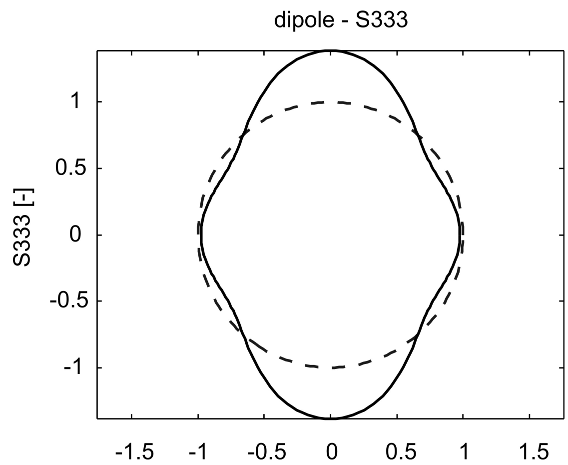

Fig. 3. Stress component S_{333}.

$$s = \frac{E_\mathrm{c}}{E_\mathrm{m}}, \tag{7}$$

where E_m is Young's modulus of the matrix which is known apriori and E_c is Young's modulus of the composite patch computed as follows:

$$E_\mathrm{c} = \frac{F\,u}{A\,L}, \tag{8}$$

where F is the total force acting on the patch computed as a sum of dipole intensities, A is the area of the patch projected onto the xy surface, u is the displacement of the patch and L is the length of the patch in x_3 direction.

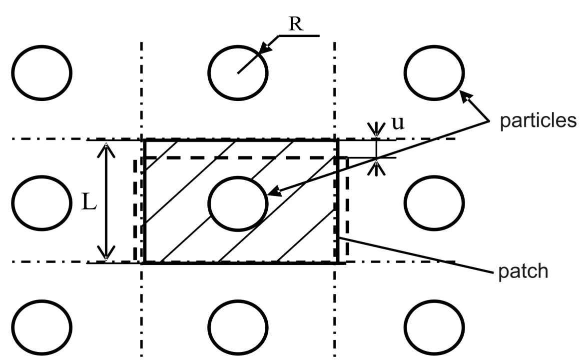

Fig. 4. Patch for evaluation of stiffening effect.

3. Results

It is assumed in the model that the particles are distributed periodically along with linear elastic isotropic material and ideal bonding between matrix and particles is considered. The Young's modulus is $E = 1000$ and the Poisson's ratio is $\nu = 0.3$. The diameter of the particles is ranging from $R = 1$ to $R = 3$.

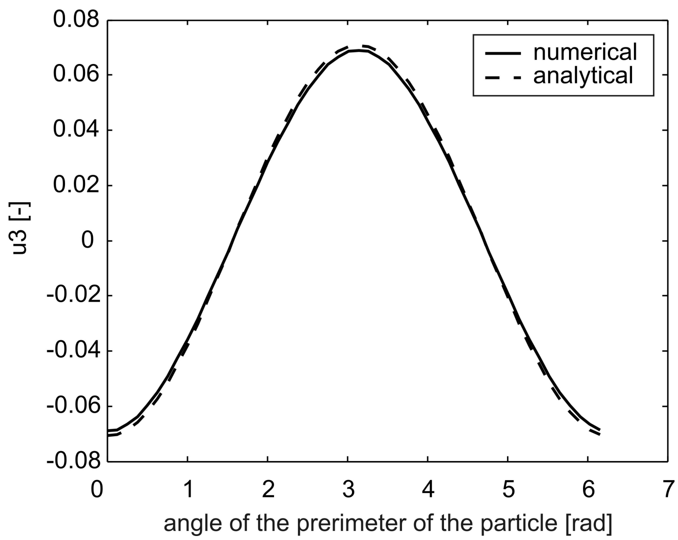

Fig. 5. Displacement u_3 of the particle.

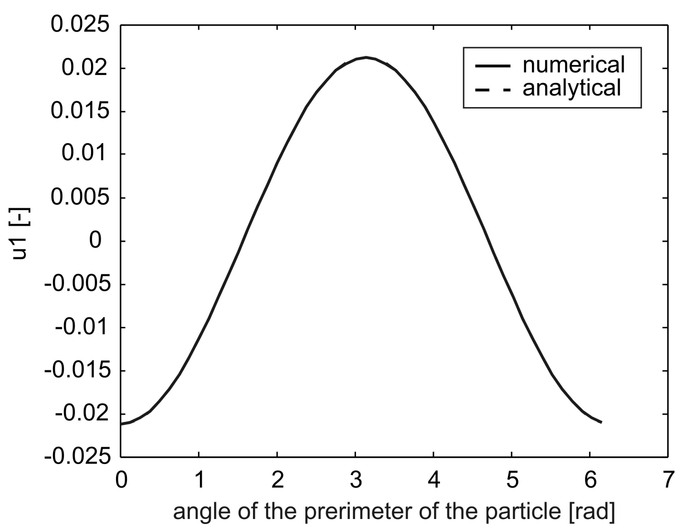

Fig. 6. Displacement u_1 of the particle.

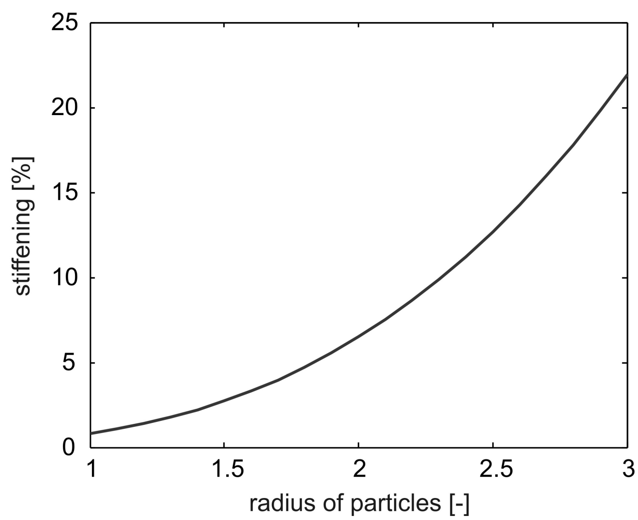

Fig. 7. Stiffening effect for different radius of particles.

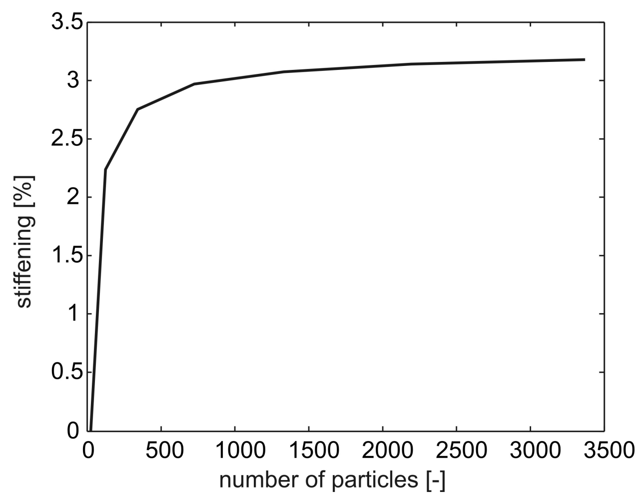

Fig. 8. Stiffening effect for different number of particles in the patch.

In Figs. 5 and 6 the deformation is shown of the particle along its boundary in the first and third direction simulated by triple dipole as compared to analytical solution (for a rigid particle).

In Fig. 7 the stiffening effect of the particles in the matrix material is shown. The stiffness is increasing with volume ratio of the particles in the matrix. Here 729 particles were equidistantly spaced, i.e. cube with 9 particles in each direction. The dependence of the number of particles in the patch on stiffening effect is shown in

Fig. 8 for radius of the particles $R = 1$. It can be seen that the stiffening converges to some value with increasing number of particles contained in the patch. For roughly 3000 particles in the patch the stiffening is more than 3 % which might be a good approximation of stiffening in infinite area given by properties of material of the matrix and shape, dimensions and distribution of the particles.

4. Conclusions

The dipole model enables to simulate both near fields and far fields in material reinforced by micro/nanoparticles and furthermore it introduces large reduction of the model compared to classical FEM/BEM methods. The shear stresses in the vicinity of the particle are important for evaluation of the strength and possible de-cohesion/re-cohesion effects. The far fields are necessary for evaluation of the reinforcing effect. The method is very simple, it does not need any elements and integration and so it is truly meshless one.

Rigid particles are assumed to be used in present models but it is possible to implement also deformable particles using iterative methods to establish force equilibrium between particles and matrix, where the deformation of the particle would be computed from the force acting on the particle boundary as a result of particle-matrix interaction.

In the case that non-uniformly distributed particles would be contained in the matrix, particles with different shapes or with different material properties or in the case that non-homogeneous material of the matrix would be assumed, the evaluation of stiffening effect would require integration of displacements and strains along the boundaries of the patch.

REFERENCES

[1] LIU, W. K.—JUN, S.—QIAN, D.: Computational Nanomechanics of Materials, Handbook of Theoretical and Computational Nanotechnology. Stevenson Ranch, Amer. Sci. Publishers 2005.

[2] LIU, W. K.—KARPOV, E. G.—ZHANG, S.—PARK, H. S.: Journal of Comp. Meth. Appl. Mech. Engng., *193*, 2004, p. 1529.

[3] LIU, Y. J.—NISHIMURA, N.—OTANI, Y.—TAKAHASHI, T.—CHEN, X. L.—MUNAKATA, H. A.: ASME Journal of Applied Mechanics, *72*, 2005, p. 115.

[4] LIU, Y. J.—CHEN, X. L.: Electronic J. of Bound. Elem., *1*, 2003, p. 316.

[5] KOMPIŠ, V.—ŠTIAVNICKÝ, M.—MURČINKOVÁ, Z.: In: Proc. of Mezinárodní konference při příležitosti založení Fakulty strojní. Eds.: Sikora, R., Zapomněl, E. Ostrava, VŠB, Technická Univerzita Ostrava 2005, p. 287.

[6] MURČINKOVÁ, Z.—ŠTIAVNICKÝ, M.: In: Proc. of the 10th International Conference on Numerical Methods in Continuum Mechanics. Eds.: Kompiš, V., Žmindák, M., Lisý, P. Lipt. Mikuláš, Academy of the Armed Forces 2005, p. 61.

[7] ŠTIAVNICKÝ, M.—KOMPIŠ, V.: In: Proc. of Technical Computing Prague Conference 2005. Ed.: Byron, P. Praha, Vydavatelství VŠCHT 2005, p. 117.

[8] KOMPIŠ, V.—ŠTIAVNICKÝ, M.: Computer Assisted Mechanics and Engineering Sciences, *13*, 2006, p. 417.
[9] KOMPIŠ, V.—TOMA, M.—ŽMINDÁK, M.—HANDRIK, M.: Computers & Structures Journal, *82*, 2004, p. 2351.
[10] KOMPIŠ, V.—KOMPIŠ, M.—KAUKIČ, M.—HUI, D.: In: Proc. of the Fifth Internat. Conf. on Engineering Computational Technology, Topping, B. H. V. Eds.: Montero, G., Montenegro, R. Dun Eaglais, Civil-Comp Press 2006, CD-ROM.
[11] ŠTIAVNICKÝ, M.—KOMPIŠ, V.—MUNJIZA, A.: In: Proc. of the COMSOL Conference Prague 2006. Ed.: Byron, P. Praha, Vydavatelství VŠCHT 2006, CD-ROM.
[12] GOLDBERG, M. A.—CHEN, C. S.: The Method of Fundamental Solutions for Potential, Helmholtz and Diffusion Problems. Boundary Integral Methods – Numerical and Mathematical Aspects. Southampton, Computational Mechanics Publications 1998.
[13] KARAGEORGHIS, A.—FAIRWEATHER, G.: IMA Journal of Numerical Analysis, *9*, 1989, p. 231.
[14] BLOKH, V. I.: Theory of Elasticity (in Russian). Kharkov, University Press 1964.
[15] KOMPIŠ, V.—KOMPIŠ, M.—KAUKIČ, M.: Journal of Engineering Analysis with Boundary Elements, *31*, 2007, p. 416.
[16] KACHANOV, M.—SHAFIRO, B.—TSUKROV, I.: Handbook of Elasticity Solutions. Dordrecht, Kluver Acad. Publ. 2003.
[17] SOMIGLIANA, C.: Sulla Teoria delle Distorsioni Elastiche. Note I e II Atti Accad Naz Lincei Classe Sci Fis e Nat, *23*, 1914, p. 463.

Received: 28.9.2007
Revised: 10.12.2007