7th INTERNATIONAL MULTIDISCIPLINARY CONFERENCE
Baia Mare, Romania, May 17-18, 2007
ISSN-1224-3264

DEVELOPMENT OF SOPHISTICATED MATERIALS USING THE COMPUTER SIMULATION

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Abstract: The paper presents computer simulation of composite materials behaviour reinforced by micro- and nano- particles and by short fibres. The computer simulation and development of computational methods specialized in nano-structures allow to development of modern sophisticated materials. The computational models enable the optimal design of reinforcing fibres for particular service conditions in order to define safe, light and reliable structures.
Keywords: multifibre composite structure, computational method, external finite element approximation, parameter, and sensitivity study

1. INTRODUCTION

Composite materials are typical with complexity of determing of mechnical properties (material parametres). Composite is heterogeneous structure that consist of two or more materials. Such way we created in macroscopic scale the third usefullmaterial with improoved properties, e.g. high strenght, stiffness, fatigue life, wear resistance, low weight etc.

Mentioned improoved properties are reason for possibility of their large utilization. For the purpose of research of composite possibilities it was developed multi scale and multi physics methods [3].

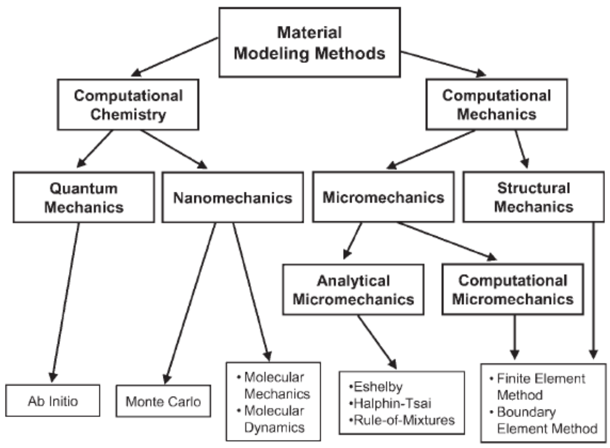

Fig. 1 *Material Modeling Methods*

Methods for modelling of material structures, according to [3, 5] are in the fig. 1.

Using the macromechnical approach, the composite structure is consider as homogeneous. The unidirectional fibrous composite is characterised by five quantities: longitudinal tensile strength, longitudinal compression strength, transverse tensile strength, transverse compression strength and shearing strenght and the composite is condider as anisotropic material. Using the micromechanical approach, the composite is consider as non-homogeneous. The matrix and fibre are modelled individualy with their own material properties

We focus on composite materials reinforced by micro- and nano- particles and by short fibres that are arrange unidirectional.

2. COMPUTATIONAL METHODS

Several authors considered continuum models with rigid inclusion to simulate the mechanical behaviour of such composites and used Finite Element Method (FEM) or Boundary Element Method (BEM) models. Recently a much more efficient solution using the Fast Multipole Method (FMM) was presented by some authors. The FMM uses the Taylor expansion (up to 10 terms) of integral equations with singular and quasi-singular terms describing the interaction of rigid inclusion with the closest neighbours and with the flexible matrix. The FMM models reduce drastically both computer time and storage requirements so that models, which were not possible to solve with present computational technique, are investigated. The method enables to solve the continuum containing up to millions of such inclusions in a supercomputer, or with clusters of computers by parallel algorithms.

Another efficient method based on integral equations is the Method of Fundamental Solutions (MFS) and new developed Method of Continuous Source Functions (MCSF) [2]. The efficiency of the methods is based on the solution, which does not need any integration. The source points are chosen outside the domain and a simple point collocation is used for satisfying the boundary conditions. However, large number of points is necessary to satisfy boundary conditions for more complicated problems.

The Method of External Finite Element Approximation [1] is used for simulation of mechanical behaviour of composite material reinforced by micro- and nano- short fibres that are arrange unidirectional

3. METHOD OF EXTERNAL FINITE ELEMENT APPROXIMATION

The Method of External Finite Element Approximation uses specific elements called subparts (cells) of arbitrary shape. Ce'a introduced the idea of external approximation in 1964. The method was developed by J. P. Aubin (1972) and by Victor Apanovich (since 1981) who was a professor at Minsk University (Belorussia). Nowadays, he is a president of Procision Analysis Inc., Mississauga, Ontario, Canada.

In mentioned method, the discrete solution space (fem space) is not a subspace of the solution space (which has infinite dimensions) therefore the method is named as „external". The domain is split in several subparts and the approximation is built on each of these subparts (independently of each other). It means that each subpart has its own set of approximation functions. Then, at the interface of the subparts, the discrete solution may be discontinuous (and therefore does not belong to the solution space). But then you can penalise these discontinuities using, for example, Lagrange multipliers and get a solution that is 'almost continuous' across the interface between two subparts. If the domain is not properly divided (you may call it meshed) then the matching of the approximations at the interfaces is more difficult.

The subpart can be called Trefftz elements since the Trefftz functions are used inside each element – subpart. The Method fulfils the governing equation exactly and boundary conditions approximately.

Comparing with classic FEM (p-version), the Method of External Finite Element Approximation uses several orders fewer elements keeping the precision. Therefore the Method has lower request for computing power.

4. APPLICATIONS

We focus on simulation of mechanical behaviour of composite materials reinforced by micro- and nano- particles and by short fibres that are arrange unidirectional using the Method of External Finite Element Approximation.

The aim is to find the principial parameters (Fig. 2) that mostly influence the strenght properties of multifibrous composite structure. Moreover, the aim is to analyze the sensitivity of structure to variation of parameters in order to design the structure for concrete service conditions.

Using the symmetry, the part of model in Fig. 2 is modelled for simulation. The matrix and fibre modulus of elasticity ratio is 1:100, Poisson ratio ν = 0.27. The model is 3D solid model without idealization. The fibre is straight and cylindrical. The end of fibre is modelled as half-sphere to avoid singularity. The applied load is tensile, uniform and defined as force per unit of area.

The model is isotropic linear consider only elastic deformation. The interface between fibre and matrix is consider as perfect therefore the fibre and matrix create the continous material. The other assumptions of simulation are homogenity, linear elasticity, isotropy and perfect straight of fibre and for matrix the homogenity, linear elasticity, isotropy, without gaps, seeds, cavities, etc.

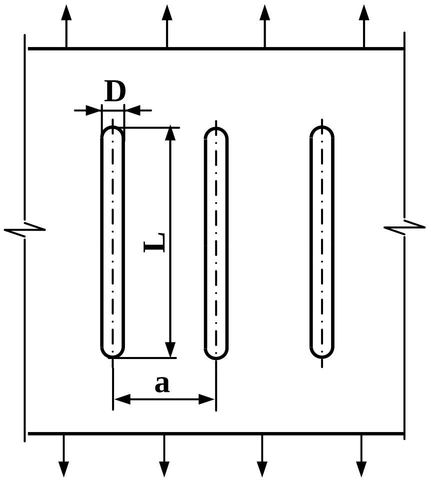

Fig. 2 *Principal model parameters*

In order to find which parameters influence the Von Misses and shear stress the most, we make the sensitivity studies. Changing the parameter, the change of Von Misses and Shear stress is monitor. The principal parameters of multifibrous composite structure are:

- axial distance a,
- fibre diameter *D*,
- fibre length *L*,
- E_f/E_m ratio.

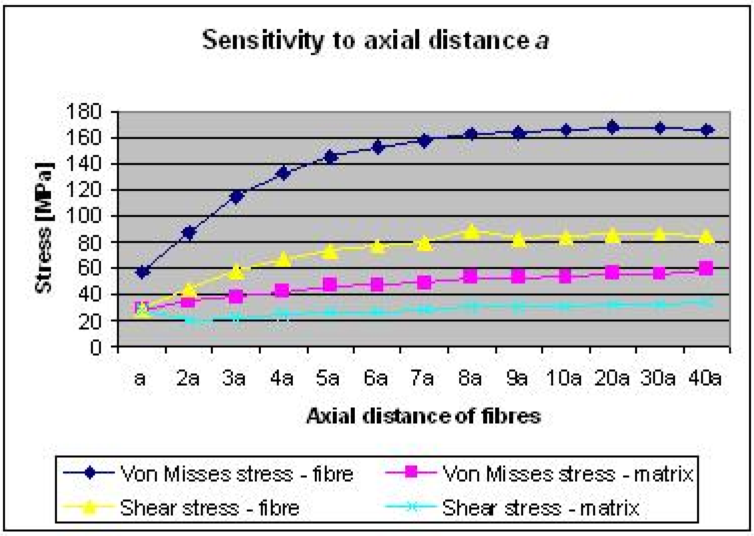

Fig. 3 *Sensitivity to axial distance a*

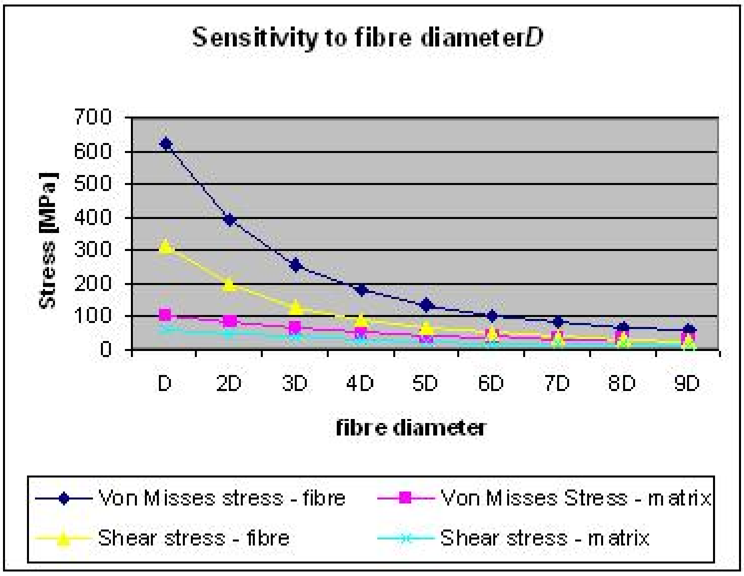

Fig. 4 *Sensitivity to fibre diameter D*

The fibre is the principal component that transfers the load. It is apparent in results of sensitivity studies. The fibre responses the most sensible to variation of each of four parameters:

1. Considering the influence of parameter *a*, we notice the evident sensitivity to axial distance of fibres by value 7*a* (i.e. 7-times fibre diameter) mainly in fibre. Von Misses stress increases 2,77 times in interval *a* – 7*a*. In interval 7*a* – 40*a*, it increases only 0,15 times.
2. Considering the influence of parameter *D*, we notice the great influence if the fibre diameter is decreacing.
3. Considering the influence of parameter *L*, we notice the longer fibre the larger Von Misses stress by the value 4*L*. In interval *L* – 4*L*, Von Misses stress increaces approximately 3 times. Elongating the fibre, Von Misses increase is not markable.
4. Considering the influence of E_f / E_m ratio, we notice the modulus of elasticity modulus increases 12 times but Von Misses Stress increases only 2.5 times.

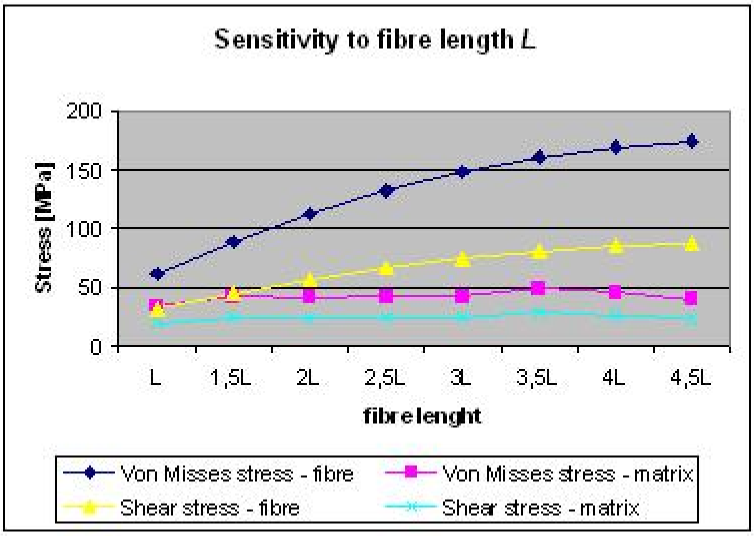

Fig. 5 *Sensitivity to fibre length L*

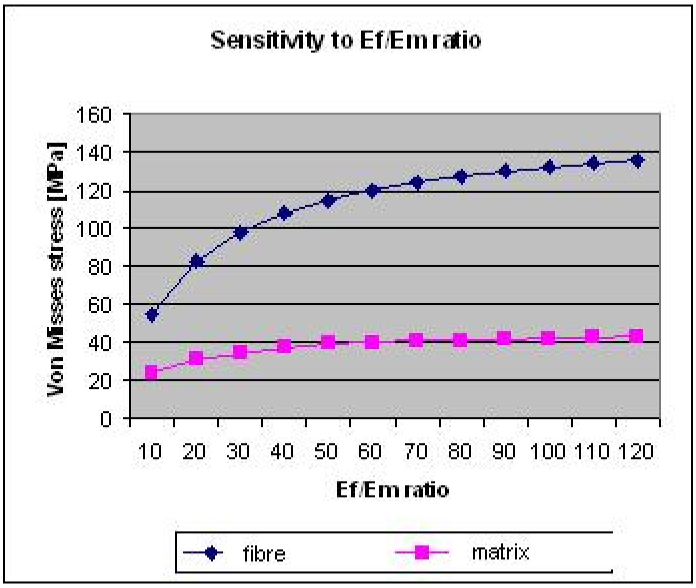

Fig. 6 *Sensitivity to E_f/E_m ratio*

Furthermore we can resume:

- the smaller fibre diameter and larger axial distance, the larger Von Misses Stress in fibre by the specific value,
- the larger axial distance, the larger Von Misses Stress by the specific value, where the increase of stress is minimal concerning the axial distance,
- the smaller fibre diameter and longer fibre, the larger stresses in fibre both and in matrix at the end of fibre,

5. CONCLUSION

Nano-structures allow the new approach in the optimisation. It requires optimisation of the length of reinforcing particles and their distribution in the matrix in order to obtain material with optimal mechanical properties. The fibres can be also curved, or have special structure (pattern) in order to improve the properties of the composite to special requirements.

Novel approach will be modelling composite nano-structures for complex applications and make-bespoken design. It is necessary to know all parametres influencing the strength of structure in order to design sophisticated material in conditions of simple or combined load. The computer simulation is very suitable and effective approach together with sufficient computational methods that are developed especially for material modelling.

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