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Abstract: The material volumes containing internal submicrocrystalline and nano structures are investigated by numerical methods of continuum and quantum

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mechanics and some computational tools have been developed. Purpose of the research is numerical multiscale modeling and computer simulation of nanoparticle-reinforced materials and carbon-like nanostructures.

INTRODUCTION

Micro-scale material property modification and modelling is already being carried out. The ability to model/predict the behaviour of materials at the micro-scale has been successfully achieved in many studies and applications. The coupled modelling at the intersection of micro and nano-scales is the primary challenge associated with hierarchical modelling of materials; namely, the accurate prediction of material properties from nanoscale to micro-scale without loss of intrinsic structural information. This can be prevented by verification of analysis methods and validation of simulations at both the atomic and bulk scales (1).

NASA researchers (2) described a hierarchical multiscale approach for modelling of materials as follows: a quantum description of materials (molecular mechanics or molecular dynamics), at the next scale, incorporating micro-scale features and simplified constitutive relationships, and further progressing up to the meso by combinations of micromechanics and well established theories such as elasticity. He says that the crucial issue of this scheme is the "handshaking" between the molecular dynamic nanoscale region and the macro-scale approaches like finite element analysis (FEA). In addition, molecular dynamic simulations are very computationally expensive for billion particles.

Continuum methods were developed for a transition from the microscale to the macroscale where the behaviour of molecules and atoms can be homogenized. A central issue of micromechanics models is the development of a representative volume element (3–5). Due to fundamental difference in computational micro- and nano-scale mechanics of composites, the models of continuum approaches cannot be directly applied to nanoscale materials (6). Continuum mechanics may be used to describe nanoparticles as components of internal structure of damping material. Thus, the methods of such multiscale transformation should be developed and verified by quasi-continuum approaches and multiscale techniques.

The quasi-continuum (QC) method (7–9) and other combined atomistic and finite-element methods (FEM) were developed. Joint finite element-molecular dynamics (FEM-MD) multiscale model was adopted to calculate mechanical properties of nanotubes and related composite materials. Despite the author's efforts the gap remained between adequate nanoscale and macroscale models.

At NASA Langley Centre, Odegard (10) has developed an equivalent-continuum model and used molecular mechanics firstly to determine at nanoscale linking forces between individual carbon atoms using a pin-joint

truss model. Li and Chou (11) improved the model by finite element analysis of the mechanical properties of the nanotubes. Damping properties was not an issue in the studies and still give a challenge for nanoparticle-reinforced materials. Thus, critical issues related to nanoparticle-reinforced materials include need to develop an affordable, reproducible computational methods and techniques to model/predict damping properties of the materials. The technology gap is a linking between micro–meso-nano-scales for dynamics/damping considerations.

This and further research work has to be carried out because we need materials that works better over broader operating ranges and is much more durable. Thus main goal of our joint team is the development, and validation of the computational tools and algorithms required to model/predict the damping properties of materials reinforced with nanoparticles/fibres/tubes etc. over broader operating ranges in frequency, amplitude and temperature.

MODEL AND METHOD OF SIMULATION

Adequate description and numerical simulation of deformation and fracture mechanics of materials at different loading conditions is important problem for design of new advanced materials. It is well known experimentally (12, 13) that plastic deformation is generated irregularly and its development is accompanied with localized strains of different length scales at prefracture stage. At meso and macro scales there are shear bands, thinning regions, Lüders bands, neck formation, etc. The subject of this paper is the problem of computational simulation of such the phenomena and computer modeling of nanoparticle-reinforced material.

An approach of mesomechanics of solids, the concept of length scales and structural levels of deformation and fracture has been used in research works (14, 15). Fundamental mechanical parameters of plastic deformation are still a chalange at mesoscale. In the present research we consider a mesovolume of material as a volume that has heterogeneity of material structure. In such a mesovolume of material the medium is non-homogeneous itself. It has a structure that evolves in loading direction. Heterogeneity of a structure can be taken into account explicitly and other non-explicitly by using some model of continuum medium. Heterogeneity of internal structure of a material may cause heterogeneity of a stress-strain state in material under loading. Main features of stress-strain state observed in experiment should be received by computational simulations.

Finite difference analysis of a model can be used to describe mesovolumes of different materials and will be carried out below. We use simple isotropic elastic-plastic model and consider an inhomogeneity of materials

at the mesolevel. Quasi-static loading is simulated by dynamic numerical method.

The Lagrange approach is used and 2D problems under plane strain and plane stress conditions were considered. A set of equations of dynamics of deformable solids for the case of two dimensional plane elastic-plastic flow with von Mises yield criterion was used (16, 17). The basic equations are the following. Equations for strain rates can be written as:

$$\dot{\varepsilon}_{xx} = \frac{\partial v_x}{\partial x}, \quad \dot{\varepsilon}_{yy} = \frac{\partial v_y}{\partial y}, \quad \dot{\varepsilon}_{xy} = \frac{1}{2}\left(\frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y}\right),$$

$$\dot{\omega}_z = -\dot{\omega}_{xy} = \frac{1}{2}\left(\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}\right),$$

$\dot{\varepsilon}_{zz} = \dfrac{\dot{h}}{h}$—for plane stress state, and $\varepsilon_{zz} = 0$—for plane strain state.

Equations of motion in plane x-y coordinates are given by:

$$\rho\frac{\partial v_x}{\partial t} = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y}, \quad \text{or } \rho\frac{\partial v_y}{\partial t} = \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y}.$$

Equation of continuity can be found as follows:

$$\frac{\dot{V}}{V} = \dot{\varepsilon}_{xx} + \dot{\varepsilon}_{yy} + \dot{\varepsilon}_{zz}.$$

Equations of state are calculated as follows:

$$\sigma_{ij} = -P\delta_{ij} + s_{ij}, \quad \dot{\varepsilon}_{ij} = \dot{\varepsilon}^e_{ij} + \dot{\varepsilon}^p_{ij}, \quad \dot{\varepsilon}^p_{ij} = \dot{\lambda} s_{ij},$$

$\dot{P} = -K\dfrac{\dot{V}}{V}$—for stresses lower than 1GPa and barotropic model of medium,

$$\frac{Ds_{xx}}{Dt} = 2\mu\left(\dot{\varepsilon}_{xx} - \frac{1}{3}\frac{\dot{V}}{V}\right) - 2\mu\dot{\lambda}s_{xx}, \quad \frac{Ds_{yy}}{Dt} = 2\mu\left(\dot{\varepsilon}_{yy} - \frac{1}{3}\frac{\dot{V}}{V}\right) - 2\mu\dot{\lambda}s_{yy},$$

$$\frac{Ds_{xy}}{Dt} = 2\mu\dot{\varepsilon}_{xy} - 2\mu\dot{\lambda}s_{xy}, \qquad \frac{Ds_{zz}}{Dt} = 2\mu\left(\dot{\varepsilon}_{zz} - \frac{1}{3}\frac{\dot{V}}{V}\right) - 2\mu\dot{\lambda}s_{zz},$$

$$\sigma_{zz} = -P + s_{zz} = 0\text{—for plane stress state,}$$

$$s_{zz} = -\left(s_{xx} + s_{yy}\right)\text{—for plane strain state,}$$

where $(Ds_{ij}/Dt) = \dot{s}_{ij} - \dot{\omega}_{ik}\, s_{kj} + s_{ik}\dot{\omega}_{kj}$ is Jaumann time derivative and $\dot{\lambda}$ is a scalar plastic flow rate parameter defined with the von Mises yield condition as follows

$$s^2_{xx} + s^2_{yy} + 2s^2_{xy} + s^2_{zz} = \frac{2}{3}Y^2_0$$

where x, y is space coordinates, v_x is velocity in x direction, v_y is velocity in y direction, σ_{xx}, σ_{yy}, σ_{xy}, σ_{zz} are stress tensor components, s_{xx}, s_{yy}, s_{xy}, s_{zz} are stress deviators, ε_{xx}, ε_{yy}, ε_{xy}, ε_{zz} are strain tensor components, P is hydrostatic pressure, $V = \rho_0/\rho$ is relative volume, ρ_0 is reference density, ρ is actual density, K is bulk modulus, μ is shear modulus, h is a plate thickness, Y_0 is yield strength. The dot over a parameter is a time derivative.

For numerical solution of this set of equations a computer program based on the finite-difference scheme known as Wilkins method was used (16–18). An algorithm of splitting of grid nodes was applied to model a fracture.

RESULTS AND DISCUSSION

The first example of simulation presents modeling of deformation of representative mesovolume of polycrystalline steel sample. A map of such mesovolume is submitted in Figure 1. There are more than 120 grains with average size about 3 microns in this volume and it can be called representative. In calculations for fragments of different color (grain) the yield strength was different (up to 30%). In uniaxial tension of such mesovolume the system of localized deformation bands take place with inclination of them about 45° to the axis of tension. In Figure 2 the greater values of intensity of plastic deformations $\varepsilon_i^{pl} = \sqrt{\frac{2}{3}}\left[\left(\varepsilon_{xx}^{pl^2} + \varepsilon_{yy}^{pl^2} + 2\varepsilon_{xx}^{pl^2} + \varepsilon_{zz}^{pl^2}\right)\right]$ correspond to greater intensity of coloring. The deformation in bands, covering on width about 0.5–0.8 microns, ranges up to 30% at integral deformation of a sample 0.7%. The system of bands of localized deformation breaks a sample into separate blocks (bulk structural

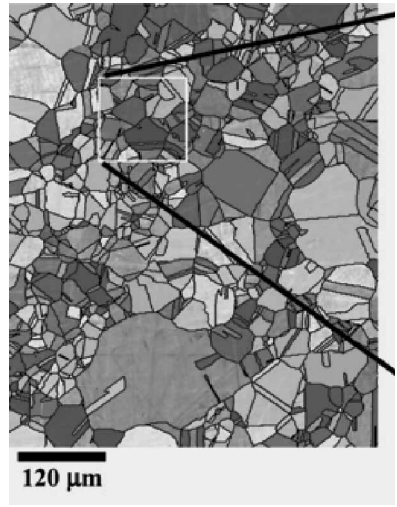

Figure 1. Map of representative mesovolume.

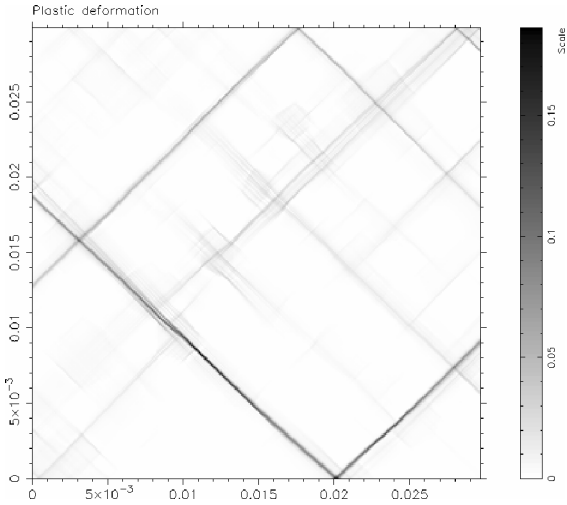

Figure 2. Distribution of plastic strains in the representative mesovolume.

elements) which move as units. This effect of material fragmentation during loading is distinctly seen in velocities field shown in Figure 3.

The later example of calculations shows deformation behavior up to failure of a ceramic composite with Al_2O_3 inclusions and Al matrix. Under complex loading (shear + tension) in a mesovolume of the composite a system of microcracks appear (Figure 4). In these calculations an algorithm

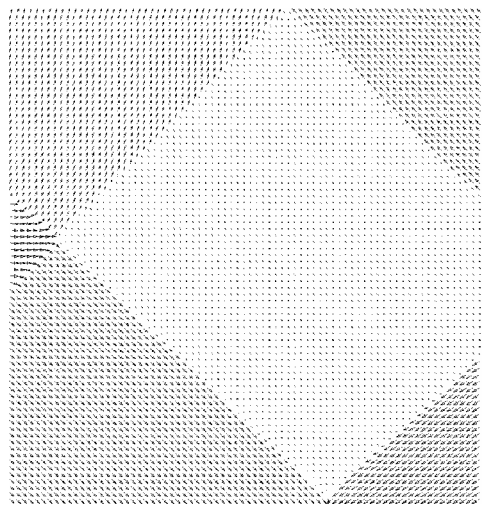

Figure 3. Velocity field in the representative mesovolume at fragmentation.

Figure 4. Mesocrack formation in the composite material with a matrix and brittle inclusions.

of Lagrange grid nodes splitting was used. Here plastic matrix transmits loading to brittle inclusions, that crack while shear bands forming in matrix.

COMPUTATIONAL AND ANALYTICAL TOOLS FOR 3D MODELING

Many of the computer calculations and simulations of composite materials carried out in computational chemistry require powerful computational resources and developments in computer science and information analysis. The software for vector and parallel computing has had great influence on material science over the last 15 years because of the hardware development of processors. It seems likely that the continued increase in capabilities of computer hardware and new software will have great impacts on the nano industry and molecular modeling.

The use of molecular dynamics in modeling of materials is one of the great applications and successes. It has been important both for material crystallography and for establishing the structures of new carbon-reinforced composite materials. However, since the X-ray experimental data in crystallography of material are insufficient to study the structure at atomic level, researchers need to use new model and approach to fill in the gaps.

The XPLOR program (19), developed by Brunger and Karplus, is by far the most popular program for combined molecular dynamics/X-ray refinement and provides a good example of the general methodology. In it, one refines the initial structure using a function that contains both the difference between calculated and observed reflections and the molecular mechanical energy function. By using molecular dynamics and high temperature, one can move the structure out of local minimum and, by changing the weights of the molecular mechanical energy and the fit to experimental reflections, guide the system to a structure that has good stereochemistry and bonding and accurately reproduces the experimental reflections.

Modeling is even more important in deriving macromolecular structures by NMR, where the number of experimental geometric data is significantly less than in crystallography (20). Thus, using various technologies to guide the determination of the 3D structure, such as distance geometry and molecular dynamics, plays a large role in NMR structure determination of macromolecules.

Improvement in computer graphics has been probably the single largest contributor to a wide use of molecularly based modeling. Although some specific history is mentioned below in the chapter on molecular modeling in the pharmaceutical industry, the ability to visualize the drug target (when its structure was known) or a conformational family of active and inactive analogs was essential in the involvement of non-modeling experts (i.e., the synthetic chemists) in the modeling. Computer graphics came of age when one could use depth cueing and stereo in color and thus highlight important interactions (21). It has continued to develop and allow ever more beautiful and imaginative representations of important processes of interest (22).

Distance geometry and computer graphics are other areas of scientific development for modeling of reinforced composite materials. The transfer of this esoteric mathematical subject to applied molecular systems was done and used by Crippen, Havel (23–25). Crippen has continued to develop it for modeling of macromolecule interactions (23).

When the structure of composite material is complex with many clusters and hard inclusions, it is essential to use computational methods that can accurately predict the structure of entire composite material and a single cluster for an entire database of computational results. The programs DOCK (25) and FLEXX (26) enable one to screen databases of the order of 100,000 clusters and screen for those most likely to bind to a target macromolecule and virtually the composite material. The other nanosimulation software is the program AUTODOCK (27), which carries out more extensive simulation of a single cluster of material using a Monte-Carlo-based method. Methods to carry out simulations are being developed (28) and should have a major impact in structure-based nanomaterials design.

Our joint group is exploring the use of spatially immersive virtual reality systems and modern IT technologies for interactive modeling and visualization of nanotechnology relevant systems. A computational scheme that

utilizes FEM-based approaches and modern software tools is used to predict/model a number of mechanical properties of nanoparticle-reinforced materials. Nanoparticle/fibre/tube etc. can be modeled by computer-vision-assisted techniques enable semi-automatic intermittent 3D graphic model update to match the simulated virtual reality of nanoscale reinforced materials with their experimental/theoretical data. In result we can easily have the 3D virtual world of the materials.

Developed software and (info/analytical tools) IT tools for modelling of virtual reality of nanoscale materials and computational approaches offer the following key features.

1. Developed a computational scheme and software utilizes FEM/BEM-based methodology and modern software simulation languages (Microsoft.Net and C#). It differs by the three-level architecture of information systems and tools for virtual nanoengineering. Main concept of the developed tools includes additional novel level of persistent nanoobjects modelled via known MatLab/C# software platform.
2. Developed a unique set of FEM-based algorithms to encode the nanoparticle-reinforced material directly into numerical vector modules that can correlate these numeric inputs with a set of desired properties. The interactive system employs a validation and optimization procedure trough a virtual three-degree-of-freedom arm and a real-time graphic display.
3. The computational tools includes a server of applications and database of Master curves based on experimental and computational results, computational tools to predict/model a behaviour of material and distance assess tools to optimize/manage the virtual solutions. The tools are easily integrated with known research platforms and databases. Thus, it would make a universal engineering logic to model/predict a multiscale behaviour of nanoscale reinforced material.
4. Developed problem tracking system is to be used for detecting, registration, processing, and localization of occurred errors or lack of data, testing, modification and modeling some possible solutions, delivery of solutions to a client or an engineer. Detected problems are classified for internal usage by an engineer.

   Software system provides for semi-automated calibration of 3D computer-generated images (e.g., "virtual reality" images) from digitized images of nanomaterials. Three-dimensional graphic models are intermittently updated through this virtual-reality calibration, which determines the scanning microscope and camera calibration parameters by using model-based, edge-matching computer-vision algorithms.

Virtual Nanoengineering: The user can easily attach his hand to an atom or molecule and maneuver it in three-dimensional (3D) space. The resulting picture (Figure 5) of material modelling shows respectively, for example, crystallise lattice of aluminium matrix, diamond nanoparticles of chosen shape

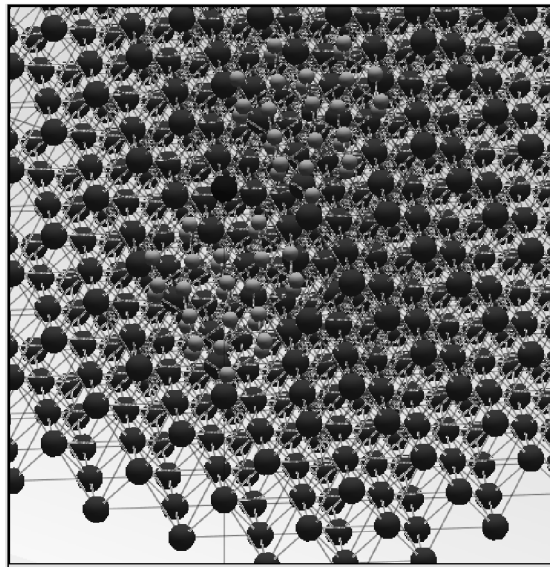

Figure 5. Nanoparticle-reinforced composite: metal matrix–carbon nanoparticles.

(pyramid-like, sphere or fullerene-like shapes) and nanocomposites represented as aluminium matrix with two introduced pyramid-like diamond nanoparticles (Figure 5). The positions of all atoms in the atomic lattices are also calculated and stored in data file. The data are used for further calculations of mechanical properties by the number of techniques (FEM, FEM, MD, etc.).

Valuable solution and tool for modelling of nanostructures and nanomaterials provide maximum performance and quality of obtained 3D video images. The reactive potential and mechanical properties are calculated from the resultant forces and motions of all atoms and nanoparticles, including changes in bonding topology. The forces on the atoms being manipulated are continuously fed back to the user through the haptic interface, while the newly calculated positions of all atoms and nanoparticles are continuously updated on the 3D graphics display.

The potential energy of the molecular systems can be calculated with the force field method. We apply the dreiding approach that is described by (29), among others. Neglecting inversion and non-bonded interactions, the potential energy of this generic force field is of the form

$$E = E_B + E_A + E_T \tag{1}$$

The bond between two atoms I and J can be described by the harmonic potential

$$E_B = 1/2\ k_e(R - R_e)^2 \tag{2}$$

which leads to the spring constant

$$c_B = \frac{d^2 E_B}{dR^2} = k_e \tag{3}$$

or by the Morse function

$$E_B = D_e\left[e^{-\alpha n(R-R_e)} - 1\right]^2 \tag{4}$$

which yields the nonlinear spring coefficient

$$c_B = \frac{d^2 E_B}{dR^2} = 4D_e(\alpha n)^2\left[e^{-2\alpha n(R-R_e)} - \tfrac{1}{2}e^{-\alpha n(R-R_e)}\right] \tag{5}$$

Figure 6 illustrates the bond stretch energies. The distance between two atoms is $R_e = 1.39\,\text{Å}$ at the equilibrium state. For the bond order $n = 1.5$, the bond energies are given to $k_e = 1050\,\text{kcal}/(\text{mol Å}^2)$ and $D_e = 105\,\text{kcal}/\text{mol}$.

The second term of dreiding

$$E_A = E_{IJK} = \tfrac{1}{2}K_{IJK}\left[\theta_{IJK} - \theta_J^0\right]^2 \tag{6}$$

describes the variation of the potential energy caused by change of bond angles, see Figure 6. This energy function leads to the spring constant:

$$c_A = \frac{d^2 E_A}{d\theta_{IJK}^2} = K_{IJK} \tag{7}$$

Alternatively, dreiding provides a cosine form

$$E_A = E_{IJK} = \tfrac{1}{2}C_{IJK}\left[\cos\theta_{IJK} - \cos\theta_J^0\right]^2 \tag{8}$$

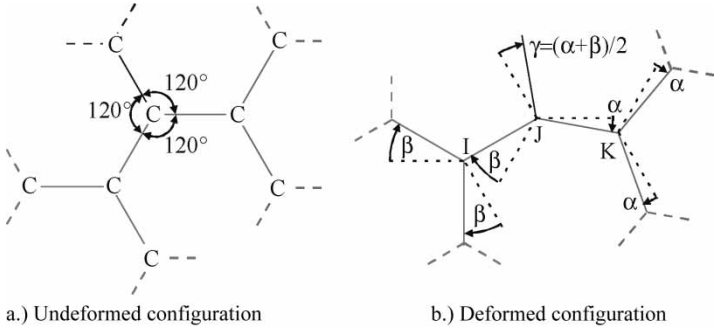

Figure 6. Bond angles.

with the nonlinear spring coefficient

$$c_A = \frac{d^2 E_A}{d\theta_{IJK}^2} = C_{IJK}\left[\cos\theta_j^0 \cos\theta_{IJK} - \cos(2\theta_{IJK})\right] \tag{9}$$

With $\theta_j^0 = 120^\circ$ and $K_{IJK} = 100\,\text{kcal}/(\text{mol}\,\text{rad}^2)$, we obtain the bond angle energies (Figure 6).

The torsion energy

$$E_T = E_{IJKL} = \tfrac{1}{2} V_{JK}\left\{1 - \cos\left[n_{JK}\left(\varphi - \varphi_{JK}^0\right)\right]\right\} \tag{10}$$

depends on the dihedral angle θ between the planes *IJK* and *JKL*. The torsional spring constant is

$$c_T = \frac{d^2 E_T}{d\varphi^2} = \tfrac{1}{2} V_{JK} n_{JK}^2 \cos\left[n_{JK}\left(\varphi - \varphi_{JK}^0\right)\right] \tag{11}$$

The equilibrium angle is $\theta_{jk}^0 = 180^\circ$, the periodicity $n_{JK} = 2$ and the torsional energy $V_{JK} = 25\,\text{kcal}/(\text{mol}\,\text{rad}^2)$.

Finite Element Models

It has to be considered that the bond angle energy $E_A = E_{IJK}$ only depends on the angle between the bonds *IJ* and *JK*. Frame elements (Figure 7a) force the adjacent bonds to rotate, but due to their bending resistance. Since this could only be prevented by additional constraints, we prefer a finite element model using spring elements (Figure 7b).

In order to be able to compute large structures containing several nanotubes, the number of degrees of freedom of the overall finite element model has to be reduced. Shell elements could be used for that purpose, see e.g., (29–32). Figures 8 and 9 show the differences between these finite element models.

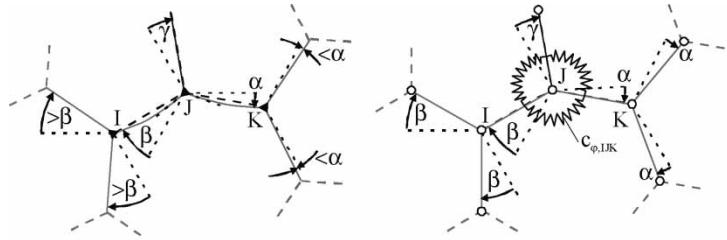

Figure 7. Simple and improved beam models.

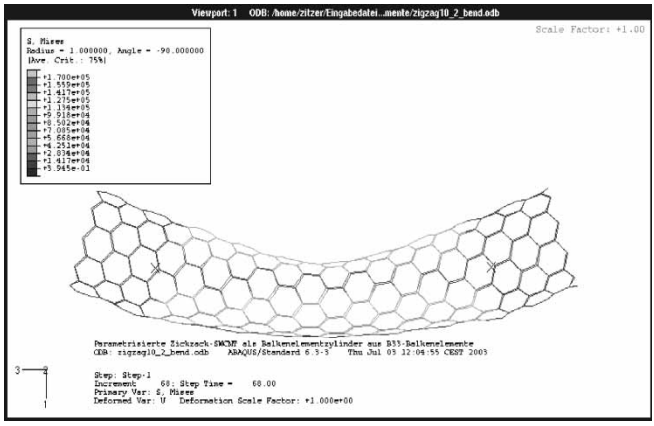

Figure 8. Beam element model.

CONCLUSIONS

It was shown the possibility of handling large gradients in displacement and stress fields by non-singular reciprocity based FEM technique using Kelvin functions with source points outside the domain. Trefftz polynomials of low order are used for the local interpolation of displacement in order to obtain the stresses inside the domain and on the domain and inclusion boundaries. The technique introduces considerable reduction of the problem. The numerical examples are shown for 2D problem; however the extension to 3D is straightforward.

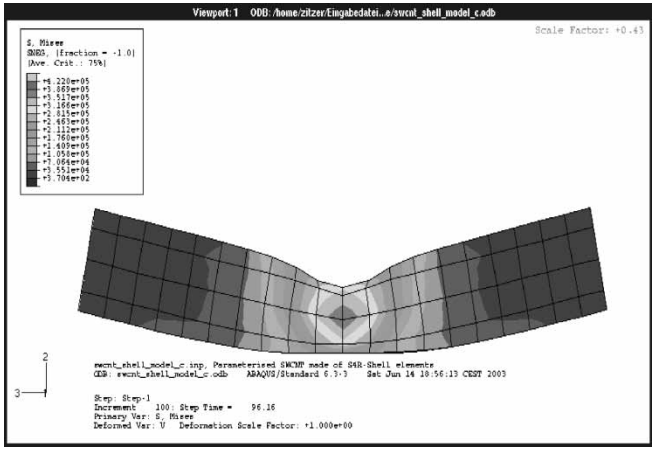

Figure 9. Shell element model.

Heterogeneity of stressed state is typical for deformation of mesovolumes of a structurally inhomogeneous material. This is due to stress concentrators of various nature and scale (interfaces of fragments of internal structure, feature of the shape, etc.). In these conditions the plastic deformation proceeds heterogeneously too. They arise in the region of stress concentration and in the least strength elements of structure. Then bands of localized shear are formed where the plastic deformations much exceed average deformations. In these bands significant change in values of shear and rotations making tensor of plastic distortion is marked, rotations being more sensitive to localization of deformation. The sign of rotations depends on orientation of a band concerning the axis of deformation. With localization of plastic deformation material fragmentation occurs with formation of bulk structural elements, which move as units. Therefore, in the frameworks of classic elastic-plastic model by taking into account the heterogeneous inner structure of a material in explicit form and stress concentrators of various nature, it is possible to simulate numerically regions of localized plastic strain of meso scale that are observed in experiments.

For a realistic simulation of the stability behavior of the reinforced material, the nonlinear intramolecular interactions between neighboring atoms have to be taken into account. A comparison shows the buckling sensitivity of different geometries. In order to reduce computational costs, it is necessary to develop suited homogenization techniques, so that shell elements can be applied.

Comparing to the FMM, the new technique will introduce further reduction of both computer time and storage requirement. Iterative solution starting from assumption that the intensity of the dipole is not influenced by the other inclusions is used in the model, will increase very efficiently computational requirements of the model solver and enable to solve problems with large number of inclusions in a PC. Although the process of verification and validation is somewhat circular, the entry point into this process is clearly through experiments that help determine the validity of theory and assumptions while also helping to quantify the state variables associated with the problem.

It is, therefore, necessary that the Computational Materials approach must use experimental data to establish the range of performance of a material and to validate predicted behaviour. Even at the atomistic level, methods such as molecular dynamics require careful parameterization (fit) to empirical data. Therein, it gives a challenge to Computational Materials: validation of methods across the complete range of length and time scales. To achieve this validation requires advances in measurement sciences as well as advances in theory and models, coupled with integrated, interdisciplinary research. It is imperative that research laboratories maintain a focused effort to develop new programs that provide for the simultaneous growth of all the critical elements that are required for validation of multi-scale methods.

While virtual nanoengineering a user can computational tools integrated with existing research database and environment via open software code integration, dot.Net and dot.COM technology. Obtained data can be treated by a number of techniques (FEM, FEM, MD, etc). Thus multiscale modeling and computational analysis of nanoparticle-reinforced materials may open a new possibility for their improvements.

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