Continuum mesomechanical finite element modeling in materials development: A state-of-the-art review*

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Advanced finite element techniques in simulation of the materials behavior under mechanical loading are reviewed. Advantages, limitations and perspectives of different approaches to the simulation of deformation, damage and fracture of materials taking into account their micro- and mesostructure are analyzed. Development of the methods of simulation of different aspects of the materials behavior (such as the unit cell approach, real structure simulation, cohesive zone model, etc) is described from initial simplest versions of the methods to advanced, highly efficient models. Possibilities of using of the finite element method in the development of new materials are analyzed. The review article contains 131 references.

1. INTRODUCTION

The development of new materials with high performances (high toughness, strength, fatigue resistance, wear resistance, etc.) becomes a very important factor of industrial progress. Whereas the achievements in the materials design have been traditionally related with discoveries of new physical effects [like skeleton from WC particles in hard alloys, which improves their compressive strength , or the globular structures of AlSi cast alloys (Mishnaevsky Jr 1995; Mishnaevsky Jr *et al*, 1999a)], and such discoveries were made mostly experimentally (i.e. by „trials and errors method"), another direction of material optimization has appeared in the last three decades (Mishnaevsky Jr *et al*, 1999b). This direction can be described in several words as follows: nowadays, most of simple physical effects (like crack growth in non-damaged material, damage growth in a non-cracked material, interface effects on deformation, interface fracture, deformation of a homogeneous material) have been well studied already and may be modeled with the use of more or less sophisticated means (like fracture mechanics, damage mechanics, plasticity theory, respectively), the synergetic interaction of these effects is becoming a promising factor of the material improvement and design.

A practical example of the application of such interaction effects in the material improvement is the "Synergy Ceramics Projects" which is carried out by a consortium of several Japanese Universities and industrial firms since 1994 (Kanzaki *et al*, 1999). The main idea of this project is "to apply the newly developed concept of Hyper Organized Structural Control to create a new family of ceramic materials". The "Hyper Organized Structural Control" includes the tailoring material properties by "simultaneous control of different structural elements, such as shape and size, at plural scale levels". In such cases, the physical mechanism of the material improvement can not be modeled with simple phenomenological models, but requires numerical simulation of the interaction between many different effects/levels in a loaded material.

In particular, deformation and fracture of real materials present extremely complex processes, which include the interaction of many objects (like different phases in heterogeneous materials, and micro- and macrocracks, which form and grow simultaneously). The numerical methods of modeling of materials, which have been developed

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* Dedicated to Prof Dr D Gross on the occasion of his 60th birthday

during the last three decades make possible the optimization of materials.

In this paper, different numerical methods of simulation of deformation and fracture of multiphase materials under mechanical loading are considered. The advantages, perspectives of development and areas of application of each of them, as well as possibilities of the use of these methods for the material optimization are discussed. Due to the author research interests, which are related mainly with the finite element simulation of strength, deformation and fracture of engineering materials, and since the FE method is the most common approach in the modeling of material behavior at mesolevel, the works in the area of finite element modeling are considered in this paper. Also, the micromechanical (in the above classification) methods, like dislocation models, nonlocal plasticity, etc are not considered here. An analysis of these methods was given by Needleman (2000).

2. COMPUTATIONAL CONTINUUM MESOMECHANICS OF MATERIALS: SUBJECT AND BASIC METHODS

Generally, the levels of the description of material behavior can be divided into nano- (atomistic level), micro- (dislocations and unit voids and inclusions), meso- (larger part of a microstructure of material, i.e. combinations of many inclusions, layers, gradients) and macrolevel (specimen). Such a classification can not be taken as exhaustive. For instance, Panin (1998) suggested even a more detailed classification, with meso-I and meso-II levels (which are defined as those related with the rotation modes inside structural elements of deformation, and those, related with the self-correlated rotations of many structural elements).

In his review of the deformation models at the mesoscale, Needleman (2000) defined “mesoscale continuum mechanics” as “intermediate between direct atomistic and an unstructured continuum description of deformation processes”. As a characteristic feature of this scale level, it was noted that “size matters” at the mesoscale. Actually, Needleman’s “mesoscale continuum mechanics” corresponds to Panin’s both “meso-I and II-levels”, and to both micromechanics and mesomechanics in the above classification. However, the themes considered by Needleman (2000) like the discrete dislocation plasticity or the nonlocal plasticity, are related more to non-continuum mechanical mesomechanics. In the present paper, the above classification will be used due to its simplicity.

Thus, the mesolevel in the material structure is defined as a range of scale levels which are 2-3 orders of magnitude greater than defects of structure (which are varied at the $10^{-9}...10^{-5}$ m scale range) and 1-3 orders of magnitude smaller than a specimen or workpiece in the following. The levels of the description can be related with some way of control of material properties: whereas the improvement at macrolevel are made only by variation of the construction of details, material improvement at micro- and mesolevel can be carried out by heat treatment, powder metallurgy means, etc.

The authors would like to suggest a generalizing term „computational mesomechanics of materials“ to designate the research works in the areas of development and use of numerical tools to study the effect of material structure on its properties and to determine the optimal structures of materials, described in this paper. The term "micromechanics of materials" which is used rather often to describe the mechanical analysis of material behavior taking into account is structure on the level of many inclusions, seems us to be inexact and confusing, since it makes no difference between mechanics of dislocations, vacancies, local interface effects, and similar microphenomena, and such phenomena as precipitation hardening, shear band localization, effect of patterns from inclusions on the strength (the simplest example – skeleton in highly filler hard alloys), etc. Therefore, mesomechanics studies quantitatively the effect of patterns of inclusions and plastically deformed matrix which influence the strength and fracture resistance of material, whereas micromechanics deals with mechanisms of formation of this patterns, damage initiation and plastic flow at the microlevel. Computational mesomechanics seeks to create the necessary numerical tools which can make it possible to describe adequately rather complex mesomechanical processes and interrelations, and can serve as a basis for material design (Raabe, 1998). In this connection, one should mention that the term "mesomechanics" has received relatively

wide acceptance recently after it has been introduced by Panin and co-workers (see Panin, 1998) as a name for the new discipline developed by them („physical mesomechanics“), the main purpose of which has been defined as the development the theoretical basis of material improvement as well, using experimental and theoretical studies of physical processes in loaded materials at mesolevel.

Methods of the mesomechanics of materials are based on solving continuum mechanics problems, which involve constitutive equations and conservation law. The solution strategies are the finite element method (FEM), boundary elements, finite differences, finite volumes, element free method, and a whole range of Galerkin type methods applicable for specific problems.

The finite difference method (FDM) is based on direct discretizing the governing equation (Fertiger, 1981; Chen, 1996). The main advantage of this method is its simplicity (both for understanding and implementation). The FDM gives a pointwise approximation to the governing equations, which discretizes the domain into a finite difference grid with nodes at intersections of the grid. Finite difference equations are established for every node. The results obtained from the FDM are "discrete", i.e. the solution in the domain other than the nodes are still unknown, which must be interpolated from the nodal values by an appropriate order polynomial function. Since the FD grids in most cases (except for some computational fluid dynamics codes like Flow3) are rectangular, this method is not very efficient in the case of complex geometric bodies.

As differentiated from FDM (which presents a domain as an array of grid point), FEM considers the domain as built up of many small, interconnected cells (elements) (Zienkiewicz, 1986). Based on the assumption that the solution region can be analytically modeled or approximated by replacing it with an assemblage of elements, the finite element method allows to obtain a piecewise approximation of governing equations.

In the boundary element method (BEM) the boundary (not all the body unlike FEM) is discretized into elements and solves for values on the boundary. The BEM is a very efficient numerical tool in the case when only the values on the boundary are of interest, while interior results are not required. The main advantage of this method is its high computational efficiency (due to the fact that BEM uses a lower dimension computational domain with regard to the problem domain), especially for elasticity problems. Brebbia (1978) has demonstrated that relationships between FEM, interpreted as a general Galerkin technique, and BEM can be established theoretically. This opens the possibility to combine both methods, when some subdomains of a considered domain are simulated with the use of FEM and others with BEM.

The discrete element method (DEM) has been developed for problems, which have to be modeled as discrete systems, due to the availability of large discontinuities comparable to the scale of problem itself. In this method, each distinct body of the system is represented by a single element, which allows for finite displacements and rotations and has contact surface with other elements (Lemos *et al*, 1985). In turn, each discrete elements may be discretized into finite elements – this approach is called “the combined finite discrete element method” (Munjiza, 1998). Although the number of degrees of freedom in the problem considered by the combined finite discrete element method is very high, this approach allows to simulate both continuous and discontinuous (fracture) material behavior.

Although many of the methods show high potential, also for mesomechanical simulations, the mainstream numerical technique for solving mesomechanical problems, which is now routinely used in most applications, remains the finite element method. This method is generally applicable for almost any continuum mechanics problem (as differed from BEM, which should be used in its classical formulation preferably in the cases when values on the boundary are of interest). Another important advantage of the FEM is its ability to formulate solution for the elements before putting them together in the entire model. This means a complex problem reduces to considering a series of greatly simplified problems (Chen, 1996; Zienkiewicz, 1986).

3 UNIT CELL SIMULATION: FROM IDEAL PERIODIC TO REAL STRUCTURES

According to Böhm and Rammerstorfer, "most

works in the field of composite micromechanics follows one of two basic modeling strategies". From these two strategies the first is the mean field analysis [which „aims to evaluate mean stresses and strains in each component of the composite“ (Böhm and Rammerstorfer, 1993)]. The second strategy, according to Böhm and Rammerstorfer (1993), is the periodic microfield approach (which is „based on detailed investigations of the microstress and microstrain distribution in „model composites“ made up of periodically repeating unit cell“ - see Böhm *et al*, 1993). One should add to this list also the direct modeling of real structures of materials which is applied widely (Wulf, 1995; Tellaeche Reparaz *et al*, 1997; Broeckmann, 1994; Mishnaevsky Jr *et al*, 1999; Hönle *et al*, 1998). The mean field analysis "averages out" all other microscale effects" (except for the reinforcement volume fraction, the aspect ratio of the inclusions and a distribution function characterizing their alignment") (Böhm and Rammerstorfer, 1993; Böhm *et al*, 1993). Thus, only two methods - unit cell model and real structure simulation - allow to take into account the real complex microstructure of materials. Consider first the unit cell approach (UCA).

The unit cell approach (UCA) has been developed from the simplest 2D version (which assumes rather specific arrangement of phases and distribution of sizes of inclusions), to complex models (which allow to simulate the behavior of multiphase materials three-dimensionally, taking into account most peculiarities of the real distribution of phases). This approach is developing now further. Fiber-reinforced composites (FRC) under transverse loading present the simplest object of the numerical simulation of the material behavior taking into account its structure: in this case, one may assume that a two-dimensional problem is solved. All classical methods of computational mesomechanics of materials, including real structure simulation, have been initially developed for or tested on fiber-reinforced composites.

In its simplest initial version, a **unit cell** model of a material presents a round fiber, surrounded by a matrix layer, and is applicable to the simulation of mechanical behavior of only fiber-reinforced composites with strictly periodical distribution of equally-sized fibers (Dong and Schmauder, 1995). In this model, evidently unrealistic assumptions about the material structure were made: absolute regularity of arrangement of inclusions, neglecting the effect of other inclusions and the matrix on the mechanical behavior of the chosen cell, etc. Yet, as shown below, this approach appeared to be very efficient in the analysis of the effect of the arrangement, volume content and shape of inclusions on the overall response of composites.

Brockenborough *et al* (1991) used a unit cell model for different periodic fiber arrangements (square edge-packing, diagonal-packing and triangle-packing) to study the effect of fiber distribution and cross-sectional geometry on the deformation (stress-strain response and stress distribution) in Al alloy reinforced with boron fibers. For random fiber arrangement they used a unit cell with many fibers. It was shown that the effect of fiber distribution on the constitutive response is stronger than that of fiber shape. Except for ABAQUS FE code (which is the mostly used FE tool in mesomechanical simulations), they used mesh-generation program QUADTREE.

Shen *et al* (1994) used plane strain and axisymmetric unit cell with cylinder, truncated cylinder, double-cone and sphere shapes of reinforcement to study the effect of shape, concentration and distribution of particles on the overall elastic response of Al alloys with SiC reinforcement; Al-Cu alloys and other composites. It was shown that the shape of reinforcements significantly effects the elastic properties of the composites. The authors have determined the forms of inclusions which ensure maximal and minimal Young’s moduli of the composites. Søvik (1996) used axisymmetric unit cell with elastic round particle and elasto-plastic matrix, and with spring elements to control stress triaxiality and analyzed the relation between stresses in particles and averaged macrostresses in AlMgSi alloys. General relation between local stresses in the particle and on continuum level was obtained.

The **unit cell with damage** [for instance, broken or debonded inclusion (Michel, 1993; Ellyin *et al*, 1993; Mozhev and Kozhevnikova, 1996, 1997) or damaged matrix (Hönle *et al*, 1998)] presents a generalization of the unit cell model for the damaged material. With the use of this version of UCA, the interaction between the material structure (properties and volume fraction of filler and matrix) and the damage initiation processes, simulate inclusion-microcrack or

inclusion-void interaction and their effect on the material behavior can be studied. In the section 5.2, this subject is discussed in more details.

The modification of the unit cell model with off-center fiber made possible to apply this model to composites with non-strict regularity of fiber arrangement (Böhm and Rammerstorfer, 1993; Böhm *et al*, 1993). Böhm and Rammerstorfer (1993) studied effect of fiber arrangement and clustering on stress fields and damage initiation in composites with the use of the square unit cell with an off-center fiber. They computed microscale stress and strain fields for periodic, modified periodic and clustered periodic fiber arrangement in Al alloy reinforced by boron fibers. Böhm *et al* (1993) used unit cell approach with perturbing periodic square array of fibers to model deterministic but less ordered fiber arrangements in Al reinforced with Altex fibers. Staggered and non-staggered arrangements were modeled by a reference volume consisting of two symmetric subcells.

Hönle (1998) studied the effects of shape, position and volume fraction of cobalt inclusion in WC/Co hard metals on the crack driving force (energy release rate) and energy consumption in crack propagation in these materials with the use of elastic and elasto-plastic unit cells with differently shaped (squared, hexagonal, circular, etc.) and differently positioned inclusions. It was shown that a growing crack is more attracted by sharp-edged cobalt inclusions and by a higher cobalt content. No notable effect of the shape of inclusion, its position in the cell or varying distance between two cobalt inclusions on the energy consumption in crack growth was observed.

The **embedded cell model** developed by Dong and Schmauder (1995, 1996) allows to avoid many of unrealistic constraints of the initial unit cell model. The embedded cell model of material presents the simple unit cell (i.e. a fiber surrounded by a matrix layer), which is embedded in some „equivalent material“. The properties of the equivalent material are determined in a self-consistent manner. The embedding allows for the effect of the rest of material and the influence of the interaction of other inclusions with a given inclusion on the behavior of the cell. The embedded cell model allows to simulate also more complex structures of materials: Leβle *et al* (1997) and Schmauder *et al* (2000) have developed the so-called "matricity model" which allows to simulate the behavior of a material consisting of two continuous phases with the use of the unit cell approach. Dong and Schmauder (1995, 1996) used the embedded cell model to study the effect of fiber volume fraction and matrix strain hardening parameters on the limit flow stress and stress - strain behavior of Al alloys with boron fibers under transverse loading. The authors have obtained stress-strain curves for square and hexagonal fiber arrangement and for different shapes of the embedded cells.

A further development of the unit cell approach is presented by the **unit cell with many inclusions** (Brockenborough *et al*, 1991; Axelsen, 1995; Axelsen and Pyrz, 1995). In this model, not regularity of an arrangement of single fibers, but rather regularity of arrangement of fiber groups is assumed. This version of UCA allows to simulate more random and more realistic distributions of fibers than the traditional unit cell models. Antretter and Fischer (1997) studied the effect of shapes and arrangement of carbides in carbide-rich regions of high speed steels with bandlike structure on the probability of carbide fracture with the use of a unit cell with two different inclusions. Different types of axisymmetric carbide shapes (generalized ellipse, polygon, „dog-bone“ shapes) under different boundary conditions (symmetric, periodic, antisymmetric) have been considered. It was shown that rectangularly or dog-bone shaped inclusions „are more likely to brake apart than those which exhibit fairly smooth and uniform stress distributions“ (Antretter and Fischer, 1997). The Weibull modulus m is shown to have a strong influence of the probability of carbide failure: for low m, the size of carbides has a main importance for their failure, whereas as m increases, the stress level inside the carbides becomes more important. The strong influence of the arrangement of neighboring carbides relative to the direction of external load was observed: depending on whether a carbide is located in the area of locally decreased stresses or in the areas of high stress concentration from neighboring carbide, the probability of carbide failure changes drastically.

Brockenborough *et al* (1991) used the unit cell with many inclusions to study the behavior of fiber reinforced composite with random distribution of fibers. Axelsen (1995), and Axelsen and Pyrz (1995) have applied the unit cell model to study

the effect of parameters of random distribution of fibers on the mechanical properties and damage behavior of composites; in so doing, the specific parameters of random microstructure (second-order intensity function, pair distribution of fibers, etc) have been taken into account. They studied the Correlation between parameters of random distribution of fibers on the stress field and crack initiation with the use of the square unit cell, consisting of sample area (with different types of random distributions of about 200 fibers) and boundary area (which interacts with the sample area, and the size of which is determined on the basis of "zone of influence" calculations). Axelsen (1995) have determined local stress fields for different fiber distributions in an unidirectional glass composite with long fibers. It was shown that clustered fibers are most sensitive toward nucleation of cracks.

Siegmund *et al* (1993) used the unit cell which consisted of an array of ideal equisized hexagons to simulate the plastic flow of two-phase alloys with different contiguities of phases. The hexagons represented grains of two-phase alloy which are randomly distributed. The authors studied the effect of contiguity of phases on the plastic flow of model two-phase material with coarse structure

In several works, **combinations** of unit cell models **with other numerical** or analytical **approaches** is used to model the behavior of material with regularity on only one scale level and without any periodicity on other levels; the behavior of such a material on different scale levels is simulated with the use of different approaches. Plankensteiner *et al* (1996, 1998), Böhm *et al* (1993), Böhm and Rammerstorfer (1993) and other members of this group have developed several very sophisticated hierarchical models in which the unit cell approach is used only at the scale at which the clear periodicity of material structure is observed; the material behavior at other scale levels is described analytically, as layered or gradient material. This approach is very close to the real structure models by the level of taking microstructure into account. To study the overall response and mechanisms of local failure of high speed steels with netlike microstructure, they used hierarchical approach, which included a mesoscale unit cell model, constructed on the basis of image analysis of steel micrographs and statistical averaging of properties at microlevel, and the transformation field approach or incremental Mori-Tanaka approach. The authors studied effect of progressive carbide cleavage on the stress-strain curve, and shown that the carbide grain cleavage is a main fracture mode at the microscale. Another approach, suggested by these authors is called Hexagonal Cell Tiling (HCT), and uses unit hexagonal cells containing a number of inclusions. This approach allows to study effect of initial thermal residual stresses on the parameters of stress distribution. The first numerical model was realized with ABAQUS, the second with the use of FE codes ABAQUS and HEXGRAIN. To study the overall response, mechanisms of damage and distribution of principal and interface stresses in high speed steels with layered structure, Plankensteiner *et al* (1998) used so-called "Micro-Meso-Macro Model". Each carbide stringer was treated as particle reinforced matrix-inclusion composite with the use of statistical averaging technique (multi-particle effective field method; Plankensteiner *et al*, 1998); at mesolevel, HSS is modeled as laminated composite. HCT-concept for the layered high speed steels uses 2D unit cell with a number of inclusions at microlevel; at mesolevel, HSS is treated as MMC with a compositional gradient. Hönle *et al* (1998) and Mishnaevsky Jr *et al* (1999) have reported also a two-level model of material behavior: the stress-strain curve was obtained from unit cell model and then assigned to each finite element in the FE model of Al/Si cast alloy; it allowed to model the damage propagation in the alloy.

Another direction of the generalization of the initial unit cell approach is the transition from 2D to 3D problems, and from the fiber-reinforced to the particle-reinforced composites. The simplest **3D version** of the unit cell model is the axisymmetric cylindrical unit cell containing a spherical void or inclusion.

Fang *et al* (1996) used 3D hexagonal and cubic unit cell with spherical, cylindrical, cubic and rectangular particles with varying orientations to study the effect of particle shapes, orientation and volume fraction on the elastic moduli and stress-strain curves of Al alloy with Al_2O_3 particles. It was shown that the higher is an aspect ratio of particles in a given direction, the more effective reinforcement in that direction.

The cylindrical unit cell allows to simulate the

material behavior under triaxial loading conditions, yet, not for the case of arbitrary stress ratio in three directions. Besides, the assemblage of such cells can not fill the space fully and therefore this approach implicitly assumes some porosity (which has been not included in the model formulation) (Kuna and Zun, 1996a). The further development in the 3D unit cell modeling is the use of prismatic and cubic unit cells (Kuna anf Zun, 1996b), which exclude the necessity of the implicit porosity assumption and therefore reflect better the real behavior of the material.

Geni and Kikuchi (1998), and Kikuchi and Geni (1998) studied effect of shapes, volume ratio, mutual interaction of particles and their spatial distribution on damage formation and strength of Al/SiC alloys with the use of a two-level model. The model included axisymmetric (cylindrical) unit cell model with elliptical particle (lower level; a model both with and without constraints was considered), and a box-shaped super element (i.e. a model, consisting of many unit cells with different particle volume fraction and shapes). The authors have obtained stress-strain relationships for alloys with different particle aspect ratio, volume fraction, availability and non-availability of side constraints, uniform and non-uniform particle distribution. Damage initiation in matrix and debonding were studied for different particle distributions as well. The unit cell consisting of many unit axisymmetrical unit cells („super element“) developed by Geni and Kikuchi, allows to take into account both non-regularity of material structure and 3D effects.

A technique similar to the above “super-element approach” was used also by Iung *et al* (1996) to compare results of the 2D (plane strain) and 3D simulations. The authors compared the stress and strain distributions in a cube and a quadrate consisting on 10x10x10 and 10x10 elements with randomly distributed properties either first or second phase. It was shown that a 2D approximation gives results which are sufficiently different from the 3D solution.

From above consideration and the results of applications of UCA, one can draw a conclusion that the unit cell approach is developing in the following directions:

- **from simple and ideal periodicity to typical (often real) microstructures of the material:** from two-dimensional round fiber-matrix unit cell to the unit cell with off-center fiber, then to the unit cells with the inclusion which presents several [also, randomly distributed; see Axelsen (1995) and Pyrz and Axelsen (1995)] inclusions with matrix. The 2D round fiber unit cell allowed to study the effect of elastic/plastic constants of filler and matrix, and the volume fraction of filler on the mechanical behavior of composite. Such cells are applicable only to the quantitative analysis of the behavior of fiber-reinforced composites or qualitative analysis of the behavior of particle-reinforced composites. Other directions are to use non-axisymmetric unit cells (the prismatic and cubic unit cells; see Kuna and Zun, 1996) instead of the fiber-matrix unit cell mentioned above, or to use "super-elements" from many cylindrical unit cells instead of the unit cells (Geni and Kikuchi, 1998; Kikuchi and Geni, 1998). These approaches can be considered as a movement from ideal to real structures as well as taking into account 3D effects. The last way allows us to simulate the 3D behavior of composites.
- **hierarchical models** appeared as very efficient approach in the description of complex structures by relative simple methods. When the periodicity and regularity of material structure is observed only on one scale level, the unit cell approach is used together with other models for other scale levels [layered materials (Böhm *et al*, 1993), "super-elements" (Geni and Kikuchi, 1998), etc].

The main disadvantage of the unit cell approach is the oversimplification: this approach requires a very high periodicity and regularity of the material structure. Actually, such materials do not exist as well as such homogeneous loading conditions. Yet, the unit cell models allow to solve (mainly, qualitatively) the following problems:

- to study the effect of the mutual arrangement of phases on the mechanical behavior of the composite,
- to clarify the mechanisms of damage initiation, or
- to study the initial stages of void formation and growth.

The advantage of this approach is that it requires relatively little computational efforts, and allows to study the complex effects in simple

computational tests. That is why many researchers prefer to use the complex combinations of unit cell models to study the complex microstructures, rather than to apply real structure simulations.

4 SIMULATIONS OF REAL MICROSTRUCTURE

A main peculiarity of the numerical simulation of particle-reinforced composites, steels and alloys, as differentiated from fiber-reinforced composites, is that the structure of these materials is always random in all three dimensions. The service properties of the materials are usually influenced by the material structures at several structural levels (like primary and secondary carbides, and network-like or layered structures in high speed steels), and only at one or two of them some regularities can be observed. Such materials can be modeled by means of the periodic microfield approach only with some losses of information about the structures. The unit cell simulation can be applicable and efficient only in the following case: the material under consideration has some periodicity/regularity in the structure, and this regularity should be one of the main factors which determine the service properties of the material. If the phases or components which influence the properties to a large extent are randomly distributed, the real structure of material should be studied. Typically, the computer description of the real structure of material is obtained through image analysis of micrographs of metallographically machined sections of the materials (Wulf *et al*, 1993; Lippmann *et al*, 1997; Plankensteiner *et al*, 1998; Mishnaevsky Jr *et al*, 1999); this is correct both for direct real structure calculations and for the approximation of material structure by the unit cell (Böhm *et al*, 1993).

The Digital Image-Based (DIB) modeling technique was developed by Hollister and Kikuchi (1994) to include the effects of microstructural morphology of bone in the FE simulations in bioengineering. FE models obtained with the use of DIB technique present direct interpretations of micrographs of composite materials. Terada and Kikuchi (1996a, 1996b) have used the DIB method together with FEM-based asymptotic homogenization method to simulate the overall mechanical behavior of composite as dependent on the geometry of microstructure and properties of components. They have shown that the actual stress-strain curve for the unit cell model obtained with the use of DIB (and reflecting the real structure) is quite different from that obtained in idealized unit cell model (elastic response more compliant, different trend of the strain hardening, etc.).

Initially, the simulations of real structure were rather intensive in modeling behavior of hard alloys and then steels (what can be explained by the wide industrial application of these materials, and evident lack of periodicity of their structure).

Consider some works in which the real structure simulations have been used. Ljungberg *et al* (1986) obtained various structures of WC-Co hard alloys from micrographs, and then idealized them to correspond the FE mesh. Then, Ljungberg *et al* analyzed the growth of the plastic zone in front of the crack as a function of the load. To model the grain/grain interfaces, the authors used so-called "nodal-tie dislocation elements". It is shown that the plastic zone size in front of the crack is much larger than the single mean free path in the binder phase. Fischmeister *et al* (1988) have studied plastic deformation of binder in front of a crack in WC-Co hard metals with the use of the FE code ASKA, and real structure embedded in homogeneous surrounding. The authors have shown that ligaments between carbides fail by nucleation and growth of pores at the points where the crack from carbides enters the ligament.

Tack (1995) simulated the deformation of coarse two-phase materials (also steels) with the use of FE-code FINEL. An element with real structure was embedded in homogeneous material with coarse FE mesh. Local refinement of FE mesh in the vicinity of hard inclusions, or in the region of a material element was carried out as well. The effect of relationships between mechanical properties of inclusion and matrix on local stress concentration, and deformation in real structure was studied.

Telaeche Reparaz *et al* (1997) simulated deformation of real structures of duplex (ferrite + austenite) steels with the use of ABAQUS. Real structures of material were reproduced by image analysis of micrographs with the use of *Verborde* and *Digit* codes. FE meshes from square elements were automatically associated with corresponding material. The authors obtained the stress-strain

curves of two-phase steel, and compared them with the stress-strain curves of components. The evolution of stresses and strains during loading was studied as well.

Carter *et al* (2000) have developed a C++-based, object-oriented FEM software (called OOF – " object-oriented finite element analysis") for the simulation of thermoelastic deformation of real microstructures of material. The software creates automatically the FE mesh on the basis of the microstructure image, and calculate stress and strain distribution in the material.

Ghosh and co-workers (see Moorthy and Ghosh, 1998; Ghosh *et al*, 1995; Lee *et al*, 1999; Li *et al*, 1999) developed a very sophisticated and efficient approach to the modeling of deformation and damage initiation in MMCs. To simulate the damage initiation (by particle cracking or splitting) in discontinuously reinforced MMCs they used Voronoi cell finite element model (VCFEM). In this method, the FE mesh is created by Dirichlet Tessellation of a real microstructure of material. Each polygon, formed by such tessellation (they are called "Voronoi cells") contains one inclusion at most and is used as a finite element.

Coupling the VCFEM for mesoscopic analysis and a conventional displacement based FEM for macro-analysis, they developed the "hierarchical multiple scale" model. In the framework of this hierarchical model, the authors use adaptive schemes and mesh refinement strategies to divide the considered volume into subdomains with periodic and non-periodic microstructures. In the periodic microstructure areas they use the asymptotic homogenization. In non-periodic microstructure subdomains, VCFEM is used.

Comparing the hierarchical VCFEM approach with the real structure simulation with the use of MPE, one may see that the first approach is ingenious, economic, requires less computational time and allows to use the regularities of microstructure to improve the computational efficiency of the model. On the other side, the MPE/real structure approach does not require any regularity in the inclusion distribution (as differentiated from VCFEM, which can be hardly used for any skeleton or clusters-containing microstructures), can be simpler generalized for 3D case and can be used to simulate both damage evolution and crack growth. Yet, current versions of 3D MPE allow to simulate only deformation of materials, not damage evolution, whereas the 3D VCFEM presented by Li et al (1999) allows to model damage initiation.

Iung et al (1996) have studied the strain heterogeneity in two-phase materials (Ti-alloys, dual-phase steels) on the basis of a developed FORTRAN program which automatically generates 2D FE mesh (to be used by the ABAQUS code) representing the image of a real microstructure. The mesh is generated "in an iterative way by superimposing on the boundaries square grid of growing size ". The mesh is refined automatically at the interfaces between the phases.

Broeckmann (1994) studied local damage and effect of local triaxiality of the strength of inclusions (carbides) in real structures of ledeburitic chromium steels with the use of the FE-Program CRACKAN. The effect of inclusion distribution on the stress state and fracture of these steels was investigated. Gross-Weege *et al* (1996) and Berns *et al* (1996) studied particle cracking, and damage evolution in front of main crack in ledeburitic steels with different states of heat treatment. The authors have taken into account also the decohesion between carbides and matrix which was supposed to occur if the stresses normal to the interface reach a critical value. A unit cell model was used as well to study the interaction between inclusions.

Common and evident weakness of the real structure simulation is the fact that each considered microstructure requires a new, very complex FE mesh. This excludes using real structure simulations in 3D case as well as in damage and fracture simulations.

Multiphase finite element method can be considered as a next step in the development of methods of real structure simulation. This method has been implemented in the FE code LARSTRAN initially; now there exists also a version of this method for ABAQUS. The main peculiarity of this method is that the different phase properties are assigned to individual integration points in the element. Contrary to the traditional (single-phase) finite elements a FE-mesh in this case is independent of the phase structure of material, and one can use relatively simple FE-meshes in order to simulate the deformation in a complex microstructure. In the case of traditional „single-phase" elements, the FE mesh should be created in such a way that the element edges correspond to

the phase boundaries, what can present some difficulties in the case of complex or fine microstructures, or even for simple microstructures in the 3D case.

The possibility of using initial meshes of arbitrary simple structures for the simulation of the behavior of complex materials is the main advantage of the method of multiphase elements. Therefore, the relatively simple simulation of material behavior in 3D case becomes possible. One should note however that MPE hardly allow to take into account fine effects of interfaces. In some cases (like WC/Co hard metals, where no real interface but rather smooth transition from pure WC through solid solutions with different concentration to practically pure cobalt is observed on interface) this limitation can be even useful and could help to reflect better the local material properties. In the cases of the materials in which no one phase is soluble in other phases, the interface presents a real boundary and impossibility to take into account the interface effects using MPE can present a serious limitation for MPE applicability.

The multiphase element method was used in several works. So, Sautter (1995), and Steinkopff and Sautter (1995) simulated large plastic deformation in Ag-Ni fiber and particle composite with the use of both single-phased and multiphase finite elements, and FE code LARSTRAN. Single-phased elements were used in simulations with hexagonal unit cell, and the multiphase elements for real structure simulation. The authors used also a rezoning technique. This technique is a „net-adaptive procedure“, like remeshing, yet, this technique does not change the net topology (as differentiated from the remeshing), but only allow controlled displacements of nodal points lying near a phase boundary in a multiphase material in such a way that the element edges correspond to the phase boundaries. For simulation large plastic deformation, the authors used repeated remeshing and Akima interpolation (i.e. a piecewise interpolation, which uses biquintic interpolation functions). It was shown that in the case of a very irregular spatial distribution of the harder phase, strain localization in the softer phase becomes less pronounced. The rotation of fibers during transverse deformation is shown to be a result of large plastic deformation in the matrix.

Wulf (1995), and Lippmann *et al* (1996a) simulated crack initiation and propagation in real structures of a multiphase material (Al-SiC alloy and AlSi alloy, respectively) with the use of MPE and the element elimination techniques (see Section 5.2). Lippmann *et al* (1996b) modeled also the crack initiation and crack distribution in high speed steels with the use of both ANSYS (with crack path predefined with the use of non-linear spring elements) and LARSTRAN (using MPE and EET). Real structure of material was reproduced by image analysis of micrographs, and embedded in the composite cell. Wulf (1995) used Rice-Tracey damage parameter and critical plastic strain as conditions of element elimination. Lippmann *et al* (1996b) used Rice-Tracey damage parameter as a condition of element elimination in matrix and critical maximum stress – in particle. The numerically determined crack path reproduced very good the experimentally observed crack path

Lippmann *et al* (1997) and Mishnaevsky Jr *et al* (1999) simulated also deformation of real structures of AlSi alloys three-dimensionally. To reconstruct 3D real structure of the material, image analysis of micrographs of many sections (cuts) of materials was used. As a result, the efficiency and applicability of 3D MPE was verified. Soppa *et al* (1998a,b) simulated the deformation of real (Al/SiC alloys) and artificial microstructures with different particle arrangement (random, arranged in stripes with clusters and gaps inside, strong and weak stripes, etc). It was shown that the more localized the particles in the stripes, the stronger the stress concentration in shear bands. The works presented by Wulf (1995), Lippmann *et al* (1996), Soppa *et al* (1998), Mishnaevsky Jr *et al* (1999) have been carried out with the use of the FE code LARSTRAN.

In order to simulate the behavior of materials with small layers of one phase between relatively large grains of the second phase, Hönle (1998) suggested to use the **mesh refinement technique**. This technique allows to adjust the element size to the thickness of layers, and to avoid the situation when the small mesh density leads to badly portrayed microstructures in the simulation. This was realized with the use of a converter, which transferred the FE mesh developed in PATRAN to FE-package ANSYS (which allows the automatical mesh refinement), and then back to PATRAN. Using this approach, MPE and the element elimination technique, Hönle (1998) calculated the crack resistance curves for real structure of a

WC/Co hard alloy. As a version of multiphase elements, functionally graded elements have been introduced by Rohde et al (1996) and Rohde (1998) to simulate the mechanical behavior of gradient materials. Similarly to the multiphase elements, the materials properties are assigned to Gaussian points, not necessarily to full elements. The assignment is made with the use of a continuum function, which allows for the gradual variation of the material properties in the gradient area.

One of recent results in the simulation of real structures is the development of a 3D multiphase finite element (Lippmann et al, 1997; Mishnaevsky Jr et al, 1999). The 3D version of MPE demonstrates the advantages of real structure simulation and multiphase elements especially clear: the regularity in the material structure can be hardly observed in 3D case (only for several very special cases, when spherical inclusions in particle-reinforced materials are not clustered), what limits the applicability of unit cell models. The construction of a FE mesh the element edges of which coincide with phase boundaries is possible only in very special cases. Therefore, a 3D MPE allows the simulation of the behavior of heterogeneous materials taking into account their structure in cases when other methods are hardly applicable. It is of interest to note that 3D MPE has been developed just several years after Poech et al (1993) predicted that „in the foreseeable future, FE models of real microstructures will have to remain two-dimensional“.

Another way to simplify the mesh generation step in the FEM simulation was suggested by Garboszi and Day (1995). They developed an algorithm to determine the effective linear elastic properties of random, multi-phase materials. The algorithm treats each pixel of the digital image of microstructure as a linear finite element. Using the digital image as the finite element mesh should simplify creating the FE meshes. The authors investigated the effective Poisson's ratio of two-phase random isotropic composites numerically and compared the results with the effective medium theory estimations. Garboczi et al (2000) and Bentz et al (1995) have used the hierarchical “multi-real structure” approach to investigate the behavior of cements and porous media. To describe the material structure at several levels, they developed a suite of models, consisting of digital-image-based structural models at the nano-, micro- and millimeter levels. Simulations carried out at one level provide input to be used in simulations at the next higher level. In so doing, the FEM simulations are combined with cellular automata –based models.

A very efficient numerical approach to the microstructure simulation was developed by Zohdi and Wriggers (1998). This methods includes the following steps: firstly, the considered area is partitioned into several subdomains with approximate local boundary conditions obtained by solving the regularized boundary value problem. The necessity of subdomain computation and correction of the subdomain sizes is verified with the use of the error estimate procedure developed by the Zohdi and Wriggers (1999a,b). If a subdomain computation is justified, the subdomain computation proceeds, using the real microstructure. The total solution is constructed then by assembling the subdomain solutions. The solution for the subdomains is obtained with the use of the adaptive FEM, which is designed to deal with general irregular microstructures. The FE mesh is automatically adapted to control the numerical error. Then the stress and strain fields for each subdomain are determined iteratively using optimal approximate analytical values from the regularized solution as a “starting guess”. The accuracy of the algorithm is ensured by the error control at each step of the simulations.

The real structure simulations expand the possibilities of computational mesomechanics significantly: whereas the unit cell models can find only limited use by definition, and any step beyond their applicability limits (what is necessary in studying the real materials) is possible only with some tricks (like looking for more and more complex symmetries in real structures of material to create unit cells with many inclusions, or creating “super-elements” from many elementary unit cells, etc.), real structure simulations allow the analysis of the effect of material structure on properties without any principal limitations.

However, the evident disadvantage of the real structure simulation is their empirism: after one carries out a simulation in a real microstructure of material, one may conclude that the used model is correct (or not), that the considered microstructure ensures high (or low) toughness or strength, etc. Yet, such a simulation can not give any

information about the preferable direction of the material improvement. Another disadvantage of the real structure simulations is that they require many computational efforts: sometimes, the shorter and more efficient is the procedure of mesh generating for a complex microstructure, the longer and more time-consuming is the simulation for this structure. That is why the optimal algorithms in the real structure simulations present a promising way to increase the efficiency of this approach.

Generally, the real structure simulations present a good basis for testing mesomechanical models, which can be then applied for the materials design.

5. MESOMECHANICS OF DAMAGE AND FRACTURE

The fracture process in heterogeneous materials consist normally on several stages: formation of voids and microcracks in random sites throughout the body, their growth, interaction, clustering, coalescence, formation of initial cracks, their growth and finally, propagation of one of the cracks up to the failure of specimen (Mishnaevsky Jr, 1996). All of these stages are strongly influenced by the inclusions and voids available in the material. Thus, the micro- and mesomechanics of fracture have to take into account all aspects of the complex interaction between crack, loaded material, and voids and inclusions in it, as well as to adapt FE procedures to the case of the growing discontinuity in the material. Most of known models take into account only some aspects of this problem.

Consider now some methods of simulation of the initiation and growth of fracture, which can serve as a basis to study the effect of the microstructure of materials on strength and fracture.

Generally, there are several main numerical techniques to simulate fracture in materials: node-release-technique, cohesive zone concept, element elimination. The main peculiarity of micro-mesomechanical simulation of fracture as differentiated from lifetime or critical load calculations, for instance, is that one may not consider the fracture only in the framework of post-processing procedures (i.e. when some parameters of crack growth or damage distribution are calculated from available stress-strain fields, and further crack growth is not taken into account). The micromechanical modeling requires the analysis of both effect of the stress field on the crack and of the crack on the stress distribution, since only such an approach may allow to study the effect of the microstructure of material on fracture. Numerical simulation of damage and fracture of materials with the use of the finite element method requires also some specific solutions in order to overcome the discrepancies between quasi-continuum statement of a problem in the framework of FEM and random, discontinuous nature of crack growth.

5.1. Damage Initiation

To model the initiation and growth of voids in materials, the **unit cell approach** (UCA) is used most often. In this paper, this subject is discussed in a separate item, however, since the problem of microcrack initiation is actually something like an intermediate step between the models of material deformation (where unit cell models are applicable in many cases, and more sophisticated versions of this approach even in most cases) and the simulation of fracture (where no assumptions about any kind of periodicity of structure may be made).

Consider some models of damage initiation in materials.

Bao (1992) simulated the effect of cracks in particles and interfacial debonding on the strength and creep resistance of composites (Al, Ti and Ni alloys reinforced with Al_2O_3). He used a three phase damage cell model (hexagonal unit cell with fractured particle; the crack plane is perpendicular to the direction of stressing; the cell is transformed into axisymmetric one), embedded into composite with undamaged particles and also a modification of this model: damage cell model with debonding at the end of cylindrical particle. Effect of total particle volume fraction, fraction of failed particles and the hardening exponent of matrix on the stress-strain behavior was studied.

Llorca *et al* (1991) studied effect of void nucleation in matrix on the deformation of Al/SiC composites (particle and whiskers reinforced) using an axisymmetric cylindrical unit cell with reinforcement of different shapes (cylinders, whiskers and spheres). To study the effect of reinforcement clustering on the deformation of composites, the authors used unit cell with different arrangements of inclusions. The authors

obtained overall stress-strain response for MMC with different reinforcement, and distributions of void volume fraction, stress and strain distribution in matrix. It was shown that the factors which increase the constraints on plastic flow (like hydrostatic stress), tend to decrease the overall strain to matrix failure.

Walter *et al* (1997) modelled damage initiation in calcium aluminosilicates reinforced with SiC fibers with the use of the axisymmetric unit cell (short and long) with fiber and matrix, which contains cohesive elements. The cohesive elements present surface elements between other continuum FEs, which can fail; the use of the elements allow to simulate the interface damage in the material. It was shown by the authors that a strong interface leads to high stress concentrations in the fiber; matrix toughness influences strongly the debonding.

Eberle and Klingbeil (1996) simulated initiation and growth of spherical voids in elasto-plastic metals with the use of cylindrical unit cell, and a modified Riks method to solve the instability problems. Effect of parameters of multiaxiality on the elasto-plastic behavior of material, local stresses, void volume and its critical level was studied. Brocks *et al* (1996) considered influence of stress triaxiality and void shape on the critical void volume in nodular cast iron on a cylindrical unit cell. The triaxiality in this work was characterized in this case by the parameter $T=(\sigma_3-2\sigma_1)/3|\sigma_3-\sigma_1|$, where σ_1, σ_1, σ_3- true principal stresses. The authors have obtained effective stress vs. strain curves and void volume fraction vs. strain curve, and determined the parameters of Gurson-Tvergaard-Needleman (see below) model from cell calculations.

Kuna and Zun (1996) studied the influence of spatial void arrangement and stress triaxiality on damage processes in nodular cast iron with the use of 3D hexagonal and cubic unit cell. The authors have shown that the spatial arrangement of periodic arrays of voids influences the deformation behavior only weakly, but affects strongly the plastic collapse. One can see that the use of the UCA makes it possible to solve the following problems: study of the effect of voids, their shape and volume fraction on the mechanical behavior of the material (i.e. stiffness reduction); simulation of particle failure, interface cracking and their effect on the stiffness of material. Sun *et al* (1996) considered the effect of distribution of microcracks and microcrack densities on constitutive response of creeping solids (ferritic steels). They used 3D hexagonal cells and tetrakaidekahedrons from power-law creeping material with penny-shaped cracks All FE simulations described above have been carried out with ABAQUS.

Mozhev and Kozhevnikova (1996, 1997) used unit cell model (cylinder matrix cell with rigid spherical inclusion) and large deformation approach to study mechanical behavior of elastomeric, particle filled composites when the separation of matrix from filler occurs. The dependence of the ultimate strength of composites on the filler content was analyzed.

Michel (1993) studied effect of particle cracking and particle debonding on void growth in matrix of Al/SiC composites using axisymmetric unit cell with ellipsoidal, broken or debonded particle. He obtained stress-strain curves for different particle shapes and broken or debonded particles.

Ellyin *et al* (1993) considered effect of biaxial and multiaxial load on damage growth in Al composites with Al_2O_3 inclusions. Using a unit cell with perfectly bonded and perfectly debonded (being simulated as contact surface) interface and FE-Code ADINA, they have shown that the interfacial layer is more easily damaged under biaxial than under uniaxial loading.

It is clear that the use of the unit cell approach in modeling of void initiation and evolution is based on a very strong assumption: namely, the voids are supposed to be more or less uniformly distributed (i.e., no localization of microcracks) and that the interaction between them is weak. This limitation may be overcomed with the use of the embedded unit cell (Dong and Schmauder 1996); in this case, the effect of other voids can be taken into account through the boundary conditions and the properties of embedding.

5.2. Damage Growth and Crack Propagation

The next stage of the damage evolution after the mutually independent void growth is the damage localization and clustering, stimulated by the local stress concentration on as-formed cracks (Mishnaevsky Jr and Schmauder, 1997a,b), and

then, the crack propagation.

Generally, there are two main approaches to the numerical simulation of fracture: a crack can be modeled as a discontinuity between adjacent elements, and a crack may be „smeared“ over entire elements (Saouma, 1995; Jirasek, 1998). Both approaches have some advantages and disadvantages: the presentation of a crack as discontinuity leads to the singularity at the crack tip, and requires frequent mesh adaptation; the smeared crack model does not exclude the stress transfer across a widely open crack in some cases (Jirasek, 1998). Methods of FE implementation of fracture models can be divided into two main group as well (one can see that these groups are naturally related with the two presentations of crack, mentioned above): methods, based mainly on special types of finite elements (Rashid, 1968; Stern and Becker, 1978) and methods which assume the specific material properties in the region of possible crack propagation. One should note that these two approaches are interrelated: models of softening of some regions, which serve as a basis in the last group of methods, require also some specific types of finite elements in this region. Among the methods of the first group, one can mention the moving-element technique (Nishioka *et al,* 1990), or triangular or brick elements with an interpolation function, which contains an inverse square root of the singular stresses; these elements are located at the crack front. As conditions of crack growth, strength or fracture based criteria (Saouma, 1995), or damage parameters (like the Gurson-Tvergaard-Needleman model for void growth model in ductile materials, see Siegmund *et al*, 1998, or continuum damage models by Krajcinovic and Fonseka for brittle materials, see Rossmanith e*t al*, 1995) are used. The criteria of void coalescence in such models of crack propagation can be based on the above described models of void growth.

Consider some methods of modeling fracture in materials.

In the **cohesive zone models** (CZM) (Tvergaard, 1997) the crack path is prescribed, and presented as a thin material layer with its own constitutive relation (traction-separation law). The relation is such that with increasing crack opening, the traction reaches a maximum, then decreases and eventually vanishes so that complete decohesion occurs. The softening part in the constitutive relation (where the traction reduces from the assumed maximal value to zero) can affect the correctness of the solution, and can result in mesh dependent FE solutions (Mishnaevsky Jr *et al*, 1998). Yet, by introducing the so-called length scale parameters into the formulation the dependence of the solution on the element size can be eliminated. Siegmund *et al* (1998) have studied interrelations between the model of crack growth based on the void evolution and coalescence (modeled with the Gurson-Tvergaard-Needleman approach) and CZM.

The **element elimination technique** (EET) is based on the removal of finite elements, which satisfy some failure condition (which is to be defined for each material to be considered). In such a way the formation, growth and coalescence of voids or microcracks, and the crack growth are simulated. As criteria of local failure, both global (external loads or displacements) and local (i.e. defined for a given element; for instance, plastic strain, von Mises stress, hydrostatic stress, etc.) values as well as any combination of these values can be used. Besides, EET can be used both for multiphase and single phase materials (in so doing, the criteria of element elimination should be chosen separately for each phase of multiphase material). To eliminate an element, all components of stress tensors in this element are set to null. As a result, all forces in this element become zero as well, and therefore, this element stops to transmit load to neighboring non-eliminated elements. The element elimination does not mean that an eliminated element is really removed from the FE mesh, yet, it stops to interact with neighboring elements. In solving the problem the tangential stiffness matrix should be corrected after the element elimination. This is done by setting the Young‘s modulus of eliminated elements to be equal to null. In order to avoid numerical problems related to strong local loss of equilibrium, the stress are set to be equal to zero in several steps (called "relaxation steps"). The Young‘s moduli in eliminated elements are set to be equal to zero in the last relaxation step. EET is incorporated in the FE code LARSTRAN (Wulf et al, 1993) and ABAQUS.

Comparing EET and CZM, one may note that the weak point in the CZM is the requirement of the crack path prescribing. Therefore, neither crack deflection, nor variations of crack path (which may

lead to sufficient variations of fracture energy, - see Broeckmann, 1994) can be described in the framework of the CZM satisfactorily. Other advantages of EET are that both microdamage and crack propagation can be simulated using the same local damage criteria. Yet, the interface fracture can be better simulated with the use of the cohesive zone model, than with the element elimination technique: in order to simulate the crack growth along an interface, one needs to introduce special finite elements or quasi-contact surface (cohesive zone, cohesive surfaces) along the interface. That can be hardly done in FE meshes automatically generated with the use of MPE.

Among approaches which are close to EET one can mention the simulation of crack propagation as a "continuum damage of material when the opening stress at 2nd Gauss point of the element in front of crack reaches a maximum value" (Wilsius *et al*, 1998).

The **computational cell methodology** (CCM), developed by Xia and Shih (1995, 1996) and Xia *et al* (1995) bears similarities both to the EET and cohesive zone model. The crack propagation is accepted to be a result of void growth in front of the crack tip. Void growth is confined to a layer, the thickness of which is equal to the mean distance between inclusions which causes void initiation. The layer consists of cubic cells, each of them contains a cavity of given size. The void growth in each cell is described with the Gurson-Tvergaard model. When the void volume fraction in a cell reaches some critical level, the cell is removed and therefore the crack grows.

A generalized formulation of the cell models of crack growth is given by Broberg (1997) in his „**cell model of material**". In this model, a material is accepted to consist on cells (which is defined as a „smallest material unit that contains reasonably sufficient information about crack growth in the material"); a cell is characterized by its size and cohesion-decohesion relation. If the cell is considered as an element in FE mesh, such an approach presents a generalization of EET, CCM and CZM models.

The cell model of material bears some fundamental similarity with the Voronoi cell approach by Moorthy and Ghosh (1998). In both cases the material is divided into "smallest" "representative" material units, different by their sizes and properties, which serve as elements in FE mesh.

The Broberg's cell model of material and the computational cell methodology allow to simulate both microcrack initiation and crack propagation with the use of one microscopic failure criterion. This is an important advantage of these methods as it is in the case of EET.

Using the cohesive zone models or computational cell methodology together with unit cells placed in front of a growing crack allows to study the mechanisms of crack growth and the effect of material structure on crack propagation. Andersson (1997) simulated crack propagation by void growth and coalescence ahead of a crack tip. He used axisymmetric cylindrical unit cell from a rigid-perfectly plastic material, with a spherical void, and varied the ratio between the size of void and the radius of the cell. The author has shown that the dissipation of energy during void growth per unit of fracture surface is proportional to the distance between voids. Using an axisymmetric unit cell with spherical void in the center of cell, Tvergaard and Hutchinson (1988) analyzed void growth in a thin ductile layer between ceramics and to determine the traction-separation law of crack growth.

The **cohesive surface model** (CSM) (Mishnaevsky Jr *et al*, 1998) presents a version of CZM. The main peculiarity of this model is that the decohesion criterion is not comprised as a constitutive law of a thin material layer joining the two parts of the system. A criterion for decohesion in this model is accepted to be controlled by the normal traction transmitted through the cohesive surface. The decohesion criterion (decohesion occurs, if the normal traction reaches a critical value) is embedded in the boundary value problem as an additional boundary condition along the prescribed crack path. The cohesive surface model allows the evolution of crack initiation from the free surface or from a pre-existing crack, crack growth and crack arrest to be described.

In the framework of the **hybrid fracture/damage approach** (HFDA) suggested by van Vroonhoven (1996), a so-called "super-element" consisting of a singular element (crack tip element) and several variable-node elements (transitional from the singular element to the linear four-node ones) is used. The element is located just on the tip of the growing crack. At the crack tip, the material stiffness is reduced 1000 times in each

timestep (the crack propagation is simulated dynamically). As a criterion of crack propagation, the J-integral (over the contour inside the super-element) was used. This approach has been implemented in the MATLAB programming environment; the FE mesh was generated with the use of SEPRAN.

The HFDA presents an alternative way to combine the simulation of crack propagation and damage growth in one model. In EET and CSM both crack propagation and damage growth are simulated with the use of the same damage model. In so doing, the crack was considered actually as a cluster of elements which were damaged (eliminated) according to the local damage criteria. In the case of HFDA, the ideas of FE models of crack and damage growth based on fracture mechanics (J-integral) and continuum damage mechanics (local failure is represented by material softening, not by discontinuity) are combined in order to avoid the disadvantages of both approaches (required frequent adaptation of FE mesh for fracture mechanics model, and mesh and damage localization sensitivity in the damage-based models).

It can be seen that the HFDA, in which a crack is simulated as a reduction of stiffness in some elements can be considered as a version of the smeared model of crack. Actually, the same is true for CZM and CCM models: in the framework of both approaches, a crack is modelled as smeared over some layer of material. The detailed review and analysis of different smeared crack models which are used often in simulations of fracture of concrete is given in by Weihe *et al* (1998). In the **smeared crack models** (Weihe and Kröplin, 1995), a crack is considered as a continuous degradation (reduction of strength/stiffness) along the process zone. The displacement jump is smeared out over some characteristic distance across the crack, which is correlated with the element size. The degradation of individual failure planes is described by the constitutive law. In the fixed crack model (Rashid, 1968), which presents the classical version of the smeared crack model, the degradation is controlled by the maximum tensile stresses only; other versions of the smeared crack model (rotating crack model, multiple fixed model) allow to take into account the variations of crack growth direction during crack propagation, and the formation of secondary cracks.

The **embedded crack model** (ECM) formulated by Jirasek (1998) seeks to combine strong points of both discrete and smeared approaches to the crack modeling by a corresponding choice of the kinematic representation of localized fracture. The idea of ECM is that finite elements with embedded discontinuity line or localization band are used. The discontinuity crosses the element and divides it into two parts. The constitutive model of the element with a discontinuity is given by both the traction-separation law and stress-strain law. This approach is similar to the multiphase elements, described above: the discontinuity of material behavior is taken into account not at the level of FE model, but at the level of the formulation of the method.

Comparing the above described approaches, one can formulate some typical features of them:

- The unit cell approach is applicable to simulate the initial stage of fracture (i.e. dispersed void formation) and to determine the criteria of local failure, which can be further used in the models of crack formation caused by the void growth. The main advantage of the unit cell approach is that it allows to take into account the effects of the material structure and stress triaxiality on the damage initiation. Thus, the introducing some results of UCA to the crack growth concepts (like Siegmund *et al*, 1998; Andersson, 1977) or relating these two concepts (Mishnaevsky Jr *et al*, 1998) can make possible to include more real physical effects in the crack growth models. If the criterion of local failure is determined with the use of UCA (instead of commonly used thermodynamical or empirical damage models), we are dealing again with hierarchical modeling.
- One of most common problems of the FE simulation of damage is the **mesh dependence**. Although it can be partially compensated by introducing special lengthscale (Siegmund *et al*, 1998), or by considering mesh size "as an independent parameter in the local approach to fracture" (Mishnaevsky Jr *et al*, 1998), this problem remains to be a basical problem of mesomechanical modeling of failure of

materials.

- In several widely accepted approaches (CZM, CSM), the **crack path** has to be **prescribed**; this presents an additional strong assumption which makes it impossible to analyze the effect of material structure on the crack propagation.
- Generally, the microstructure of material is taken into account only in several models of fracture (EET, some unit cell models), although it remains one of the main problems of mesomechanics. The use of UCA to determine the local damage parameter could allow to take into account the filler/matrix properties and volume fraction of particles also in the framework of crack growth models based on the void growth. Combining the numerical methods of simulation of deformation of material taking into account their microstructure, and the methods of modeling of crack growth should be one of main directions of further development of numerical models of fracture, and can serve as a basis for the improvement of fracture resistance of materials. One can see that growing amount of projects are planned and carried out in this direction (BE approach – see Leggoe *et al*, 1996; Bush, 1997; EET and MPE model – see Wulf, 1995; Mishnaevsky Jr *et al*, 1999a).
- One can note that both structure of multiphase materials and formation of cracks can be very efficiently taken into account by using special elements with „embedded interface“ (multiphase elements) and embedded cracks. One may suppose that the inclusion of discontinuities of materials in FE models at the levels of finite elements (and not by the means of the development of special models) can present a very efficient way to simulate real materials.

6. OPTIMIZATION OF MATERIALS

In this section, the research works in the area of materials optimization by varying their microstructures are considered to compare the efforts and achievement in the areas of materials modeling and materials improvement.

The recommendations for the improvement of mechanical properties of materials can be divided into two main groups: those, which are seeking to influence the strength (overall response, hardening, flow strength) and stiffness of materials, and those, which seek to influence the fracture toughness and resistance.

Consider firstly the first group of investigations. Bao *et al* (1991) simulated numerically the effect of aligned, uniformly distributed non-deforming particles in ductile matrix on the overall response of material. It was shown that very different shapes of particles (discs, cylinders, needles) have roughly the same reinforcing effect on the elastic-perfectly plastic matrix when the particles have random orientation. High aspect ratio needles or discs was shown to be more effective reinforcements than spheres. At a given aspect ratio, aligned needles are somewhat more effective than aligned discs.

Christman *et al* (1989) have shown on the basis of FE simulations of deformation of MMC that the uniformly distributed aligned cylindrical particles present more effective reinforcement than spherical particles

Zahl and McMeeking (1994) simulated numerically the interfacial effects in MMCs with reinforcement. It was shown that the flow strength varies with changing of interfacial properties as follows (in decreasing order): strong interface – shearing, but strongly bonded normal interface – strong interface on inclusion sides and debonding on inclusion ends.

Llorca *et al* (1991) simulated the deformation of Al alloys with SiC reinforcement. The authors concluded that the strain hardening and flow strength are maximum for whiskers and minimum for spheres shapes of reinforcement, but the strain-to-failure is maximum for the sphere- and small for whiskers- reinforced composite; the particulate reinforcement impart maximum strength, and the middle strain-to-failure. These authors have shown also that the vertical clustering of whiskers lowers the overall flow strength and promotes a slower rate of voids as compared to the uniform arrangement. Vertical clustering leads to the smaller hardening exponent and larger ductility as well, but the difference with uniform arrangement is smaller. The influence of reinforcement clustering is significantly less pronounced for particulate and sphere-reinforced composites, than for the whiskers- reinforced composites.

Böhm *et al* (1993) have shown that overall response of fiber-reinforced composites to axial loading is nearly independent on the fiber arrangement, whereas the elastic moduli and yield limits under transverse loading decrease in the following sequence: periodic square array in the 0o direction – periodic hexagonal arrangement - periodic square array in the 45^o direction.

Fang *et al* (1996) have shown on the basis of their simulations, that the higher an aspect ratio in given direction of a composite, the more effective reinforcement of composite. The work-hardening rate and effective elastic moduli vary with variation of the reinforcement shape as follows (in descending order): rectangular parallelepiped particles – cylindrical, cubic – spheres.

Soppa *et al* (1998) simulated the deformation of artificial microstructures of metals with non-metallic inclusions, and shown that the stronger the particles are clustered, and localized in layers, the greater are the shear localization and stress concentration.

One can notice some general features of the above models: they use very idealized models of materials (mostly, two-dimensional unit cell models); they all are based on numerical simulation (although we collected the recommendations independently on the used analysis) (however, one can see that such structures as „periodic square array“ or „rectangular parallelepiped particles“ can be hardly produced experimentally).

In a number of investigations the authors seek to improve the fracture resistance of materials. One may note that the recommendations given below are related mostly to different materials; yet, some common tendencies in the material development may be observed as well.

Evans *et al* (1977) and Evans (1997) studied the damage and fracture mechanisms in high temperature engineering ceramics and ceramic matrix composites. They recognized the following ways of to increase the toughness of the materials:

1. Controlled microfracture (i.e. the material contains brittle second phase particles which fail in the stress field of a growing macrocrack and therefore increase the energy consumption in the crack propagation). This approach does not lead to the increase of fracture strength.

2. Ductile second phase network. “Cylinder” particles of ductile second phase (practically, it can be realized as continuous network of ductile phase along grain boundary triple points) are better reinforcement than the spherical second phase particles.

3. Frictional toughening (which is achieved in materials containing strong aligned reinforcements with weak interfaces, which enable debonding and allow dissipation by internal friction). This mechanism is more effective than ductile phase toughening (which is achieved by ductile reinforcement in an elastic matrix).

Raj and Thompson (1994) studied the behavior of Ni/Al2O3, Pb/ MgAl2O4, WC/Co and other composites theoretically as well. It was shown that fracture toughness of MMC with continuous network from precipitates (like WC-Co, Al-Al, produced by liquid phase sintering or Lanxide process) is much higher than that for dispersed particles (fabricated by hot pressing of powder mixtures of metal and oxide followed by reduction of oxide into metal). Chermant and Osterstock (1979) and Luycks (1981) have demonstrated that the fracture toughness of WC/Co hard alloys increases with decreasing contiguity

Watanabe and Kawasaki (1992) studied functionally gradient metal-ceramic sintered (also hot pressed and HIP) composites experimentally, and have discovered two ways to increase the fracture resistance of materials:

1. Increasing the connectivity of the metal phase (Betty number) leads to the increase of fracture toughness

2. Crack arrest function of FGM is improved by metal fiber premixing in the ceramic-rich region.

Mishnaevsky Jr *et al* (2000a,b) simulated the crack propagation in high speed steels (HSS) which were considered as two-phase materials of primary carbides and “matrix”. They used multiphase finite elements and element elimination technique. The authors simulated first the crack growth in real microstructures of HSS, in order to verify the used approach. Then, they simulated the crack growth in artificial, computer-designed microstructures of the steels, with band-like, net-like and random distribution of carbides, of different sizes. On the basis of the simulations, the specific surface energy, fractal dimension and roughness of fracture surface were determined numerically.

The authors observed the following effects which increase the fracture toughness of the materials:

- crack deflection by the carbide layers oriented perpendicularly to the initial crack path (observed in the net-like coarse microstructure, band-like microstructures),
- the crack follows the carbide network (net-like fine microstructure), and
- damage formation at random sites of the steels and following crack branching (random microstructures).

Mishnaevsky Jr *et al* (2000) have shown, that the fracture resistance of steels increases generally in the following order: band-like → random → net-like microstructure. Some interrelations between the geometrical and energy parameters of fracture were observed as well: it was shown that the fracture toughness increases with increasing fractal dimension and height of the roughness profile of the fracture surface.

Tan and Yang (1998) considered nano-composite alumina ceramics with dispersed Si nano particles analytically. It was shown that higher toughness of nano-composite ceramics is achieved by particles distributed within the matrix grains along grain boundaries. Three toughening mechanisms were identified:

1. „switching from the intergranular cracking to the transgranular one“ (by nano-particles distributed along the grain boundaries),
2. „fracture surface roughening by zigzag crack path“ (by the fluctuated residual stresses from the nano-particles within the grains), and
3. „shielding by clinched rough surfaces near the crack tip“.

Sigl *et al* (1988) studied analytically and numerically brittle materials reinforced by a ductile phase (Al_2O_3/Al and WC/Co composites). They have shown that high toughness of the materials can be achieved by reinforcement of brittle materials with ductile phase with a large uniaxial work of fracture and large mean strain for hole initiation, especially in conjunction with compressive residual stresses in the matrix.

Broeckmann (1994) and Gross-Weege *et al* (1996) studied numerically and experimentally the damage and fracture in ledeburitic chromium steels. It was shown that fracture toughness of steels can be increased by

1. increasing the width of crack path (in the hardened and low tempered states) (this is achieved by increasing the cell size in netlike structure of steels, or by using netlike structure instead of band-like structure of steels) ;
2. increasing the part of crack path through ductile matrix (in the soft annealed states) (is achieved by increasing the matrix ductility, for instance, by increase in the temperature of tempering).

On the basis of their numerical and experimental investigations, Berns *et al* (1998) have developed a new material with „double dispersion“ microstructure (i.e. the coarse hard phase is replaced by a dense dispersion of small carbides), which ensures sufficiently higher fracture toughness and lifetime, and comparable with usual materials for cold forging tools wear resistance and bending strength.

Holmes and Chermant (1993) studied experimentally creep resistance of fiber-reinforced ceramic composites. It was shown that the creep resistance of composite is greater when the creep mismatch ratio (CMR= creep rate of fibers divided by that of matrix) is less than unity (it assures periodic fiber fracture mechanism of damage) than when CMR > 1 and damage formation proceeds by the mechanism of matrix fracture and bridging fibers. This conclusion is however not applicable for high monotonic toughness, since in this case matrix fracture and interfacial debonding are preferable damage modes.

A very promising way to improve the toughness and strength of materials is the using of the interrelations between phase transitions in loaded solids and the strain state. So, steels with high ductility and tensile strength can be developed using the transformation induced plasticity (TRIP) phenomena which accompanies the martensitic phase change in ductile materials (see Diani *et al*, 1995; Fischer *et al*, 1996; Reisner *et al*, 1998; Levitas *et al*, 1998).

As can be seen from above consideration, among the main ways of increasing the fracture resistance of multiphase materials one can mention:

- adding second phase particles or network, which cause accompanying, energy-consuming processes during crack growth in the first phase (matrix) (like friction, additional

microcracking, etc.), and therefore increases the fracture toughness of the material;

- creating such an arrangement of inclusions that a growing crack deflects most frequently from the path which it would follow in a homogeneous material (like the pure matrix) (this is achieved by ductile inclusions, like metal fiber premixing in the ceramic-rich region (Watanabe and Kawasaki, 1992), or weak interfaces (Evans, 1997) , or special arrangements of particle clusters; for instance, in tool steels it is achieved through netlike structure of carbide rich regions);
- varying degrees of networking (positive effect on fracture resistance) and connectivity of hard and ductile inclusions (negative versus positive effect).

Strength of the materials, as differentiated from their fracture resistance, increases with decreasing the size of the grains of ductile matrix (Mishnaevsky Jr *et al,* 1999a). The elastic constants of the material increase with increasing the aspect ratio of the reinforcement composites (Fang *et al,* 1996).

From this analysis the following conclusions can be drawn:

- Along with the chemical and microscopical methods of improving mechanical properties, there exists the mesoscopical way to do it: namely, the mechanical properties of materials can be improved by varying distribution and arrangement of phases in two-phase materials, without changing the properties of phases.

7. CONCLUSIONS

On the basis of the above consideration of some recent results in computational mesomechanics of materials, one may formulate some conclusions about perspectives of development and application of the considered numerical methods and ways to create the methodology of computational material design.

Consider firstly at some perspectives of the further development of the computational methods of mesomechanics.

Considering the application of the unit cell models, one may note the following tendencies:

- more complex, non-regular constructions of unit cell which approach to the real structures of materials (off-center unit cells, unit cells with debonded or broken particles, or with several particles),
- hierarchical or many-level modeling, super element or layered or network-like combinations from unit cells, unit cell with self-consistent embedding or, reversely, inclusion, which have properties, averaged over some volume of material or some amount of inclusions, etc.

Actually, one can say that the unit cell approach is developed from the model of a specific material with absolutely periodic structure to the approach which will be applicable for any material with at least minimal degree of regularity.

The real structure simulation which is very effort-consuming by definition has made an important step of development from single-phase finite elements (which allows to model only simple 2D real structures) to the multiphase elements which make possible to simulate also materials with complex and three-dimensional structures without enormous efforts required to create the FE mesh with all element edges along phase boundaries. In future, the real structure simulation can be used to simulate the behavior of materials without any observable regularity of structure or with structure irregularities which determine the material behavior more than regular patterns. Another, very important area of application of real structure simulation in future is the study of effect of the material structure on parameters of fracture: clearly, that there is no regularity or periodicity of properties in the material with large crack.

The **hierarchical modeling**, which was mentioned above in connection with the tendencies of development of the unit cell approach, opens also an additional possibility which presents a very perspective way of development of models of materials, namely,

- incorporating **physically based micromodels of materials** in the mesosimulation of material behavior (micro-meso-simulation). Among the models based on this approach, one can mention the **FEAt** (Finite Element - Atomistic Coupling: an atomistic region is surrounded with a finite element continuum. To overcome the different definitions of forces in the local continuum and in the non-local atomistic regions, a transition region is introduced, where the atomistic and continuum regions overlap, FE nodes correspond to atoms one-to-one and they are coupled by mutual

displacement boundary conditions**)** (Fischmeister *et al*, 1989) and the **crystal plasticity modeling** (material is presented as consisting of grains or single crystals each of them has its own lattice orientation and geometry of slip system; this makes possible to take into account the effect of different crystallographic orientations on the material behavior) (McHugh *et al*, 1993).

As can be seen from the above analysis of the simulation of damage and fracture, the processes can be modeled by one of the following ways:

- the stresses and Young‘s moduli in the finite elements in which high local stress concentrations take place are set to zero (EET, CCM);
- reduction of material stiffness in a layer along which the crack is assumed to propagate (CZM, fictitious crack model);
- the assumed path of growing crack is presented as a contact surface (CSM, unit cell model suggested by Eberle and Klingbeil, 1996).

The weakest point is the cohesive models of fracture (CSM and CZM; also CCM) is that the crack path in those models (or at least in the versions of these models available today) must be prescribed. This idealization (similarly like the assumption about the periodicity of material structure in the unit cell approach) limits strongly the possibility of use of these models for design of high fracture-resistant materials. However, a similar problem has been available in the fictitious crack model and is solved successfully with the use of the multiple fixed crack, and later, adaptive fixed crack model (Weihe and Kröplin, 1995). Therefore, one of the directions of further development of these models is to avoid the prescription of crack path, what would allow to take into account the effect of material structure on crack growth. In this connection, the element elimination technique opens outstanding possibilities of simulation of both void formation, growth and crack propagation; in so doing, the real structure of material is taken into account. This method allows to study the effect of the material structure on the crack path and fracture resistance of material, and therefore, can serve as a numerical basis for design of materials with high fracture-resistance.

On the basis of the above analysis, one can formulate a possible scheme of the optimization/design of materials on the basis of the methods of the computational mesomechanics, which includes the following steps:

1. Basical Steps:

- Analysis of the effects of material manufacturing and processing on microstructure on the basis of experiments, thermodynamical methods, etc. Example: effect of duration and temperature of sintering on grain size and contiguity of hard alloys; effect of hot working on the type of structures in high speed steel
- Definition of necessary properties to be improved on the basis of the analysis of service conditions of the workpieces from the considered material.

2. Material analysis

- Image analysis of the material structure (digitizing micrographs from cuts of the materials)
- Search for regularities or periodicity in the microstructure
- Determination of damage mechanisms in the material (debonding, particle failure, etc.)

3. Mesomechanical simulation

If the structure is periodic (like FRC), or fully random or localized, one studies the effect of material structure on the constitutive behavior (with UCA for periodic structures, or RSS for nonperiodic structures),

- Most probable case: if there is a regularity only at one scale level, and random structure on other scale levels (like high speed steels with network structure from carbide bands and random carbide distribution in bands), one needs to develop an hierarchical model of partially regular structures: UCA in combination with statistical methods, averaging methods, gradient material models, etc.
- If the damage and fracture resistance of the material has to be optimized as well, one uses UCA with damage (if the damage initiation determines the lifetime of the specimen), or simulate crack growth with the use of one of above methods.

- Optimization of structure, production and testing of the material with optimal structure

The suggested approach, by the author's opinion, can serve as a general basis for the improvement and design of structural materials taking into account their real structure. Yet, as can be seen from above considerations, the typical path of the material improvement remains to be a phenomenological/experimental/analytical way: namely, some assumptions about a possibility of material improvement are made on the basis of experiments or general physical principles, are tested experimentally, and optimized on the basis of the phenomenological or analytical models. One should note that such works where reality-close simulations and experiments allowed to improve a material, are still rather an exception.

One can see that the works on the improvement of methods of simulation of material behavior taking into account the microstructure and those which seek to improve real materials are developing rather separately and parallelly. Yet, it can be expected in nearest future that simple qualitative means of the materials improvement will be exhausted. The numerical techniques are developing in such a way that they allow efficient simulations of materials behavior taking into account real microstructures. The necessarity to optimize materials on many parameters (like fracture resistance and flow strength and wear resistance, for example) taking into account the interaction of many microstructural effects (like different failure mechanisms in different phases, deformation, clustering effects, etc.) simultaneously will cause the numerical (first of all, FEM) methods to be the main mean of material improvement.

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SOME ABBREVIATIONS:

BE	-	boundary element
CCM	-	computational cell methodology
CSM	-	cohesive surface model
CZM	-	cohesive zone model
EET	-	element elimination technique
FE	-	finite element
FRC	-	fiber-reinforced composites
HCT	-	Hexagonal Cell Tiling
HFDA	-	hybrid fracture/damage approach
HSS	-	high speed steel
MPE	-	multiphase finite element method
MMC	-	metal matrix composite
UCA	-	unit cell approach
VCFEM	-	Voronoi cell finite element model