Advanced Finite Element Techniques of Analysis of the Microstructure-Mechanical Properties Relationships in Heterogeneous Materials: A Review

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Recent advances in the numerical modelling of strength, deformation, damage and fracture of heterogeneous materials are described shortly. The areas of applicability, advantages and perspectives of different approaches to the simulation of material behaviour under mechanical loading taking into account the micro- and mesostructure of material are considered. The possible scheme of application of the computational methods of mesomechanics of materials to the improvement of material properties is presented.

1. Introduction

Control and improvement of mechanical properties of engineering materials is an important problem for many branches of industry. Such control can be achieved through changing the material structure [1-2]. As examples of the improvement of material properties, based on the changing material structure, one can mention the skeleton from WC particles in hard alloys (which improves the compressive strength of the alloys [3]) or the globular structures of AlSi cast alloys [4] (improves the fracture resistance). The information about physics and mechanics of material behaviour under loading, which have been obtained by many scientists as results of their experimental and theoretical works, may serve as a basis of the improvement of materials. The 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) ; that is why analytical methods of modelling of material behaviour do not allow to optimize the material structures. The numerical methods of modelling of materials, which have been developed during last decades make possible the optimization of materials. In this papers, different numerical methods of simulation of material behaviour 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 modelling of material behaviour at mesolevel, the works in the area of finite element modelling are considered in this paper.

In this paper, the numerical simulation of mechanical behaviour of materials at **mesolevel** is considered. The mesolevel in the material structure can be defined as a range of scale levels which are sufficiently greater than defects of structure and sufficiently smaller than a specimen or workpiece.

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 behaviour taking into account ist structure on the level of many inclusions, seems us to be unexact 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 pattents from inclusions on the strength (the simplest example – skeleton in highly filler hard alloys), etc. Roughly speaking, 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. 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 [6] as a name for the new discipline developed by them („physical mesomechanics“), the main purpose of which has beed 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. Although damage models (see [5], for instance) are mesomechanical as well both by the definition of „mesomechanics“ and by the physical meaning of damage growth processes (i.e. micro- and macrocracks are formed as a result of the interaction of dislocation movement/formation and stress field in loaded material), these models are not considered here since the theme of damage modeling is very complex and requires a special consideration.

2. Numerical Methods of Computational Mesomechanics of Materials

Böhm and Rammerstorfer wrote that "most works in the field of composite micromechanics follows one of two basic modelling strategies": mean field analysis (which „aims to evaluate mean stresses and strains in each component of the composite“ [7]) and 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“ [8]). One should add to this list also the direct modelling of real structures of materials which is applied more and more widely [9-12]. According to Böhm and Rammerstorfer, 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") [7]. Thus, only two methods - unit cell model and real structure simulation - allow to take into account the real complex microstructure of materials. Let us first consider the unit cell approach (UCA).

2.1. Unit Cell Simulations

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 behaviour of multiphase materials three-dimensionally, taking into account most peculiarities of the real distribution of phases and this approach is developing now furtherly.

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 behaviour of only fiber-reinforced composites with strictly periodical distribution of equally-sized fibers [13]. 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 behaviour of the chosen cell, etc. 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 [7-8]. The **embedded cell model** developed in [13-14] 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 behaviour of the cell. The embedded cell model allows to simulate also more complex structures of materials: Leßle et al. [15] have developed the so-called "matricity model" which allows to simulate the behaviour of a material consisting of two continuous phases with the use of the unit cell approach.

The unit cell with damage (for instance, broken or debonded inclusion [16-19], or damaged matrix [12]) presents a generalisation of the unit cell model for the damaged material.

Table 1. Simulation of Mechanical Behaviour of Fiber-Reinforced Composites

Problems	**Numerical approach and used codes**	**Main results**	**Materials considered**	**Refs.**
Effect of fiber distribution and cross-sectional geometry on the deformation of MMC	ABAQUS, mesh-generation program QUADTREE. Unit cell model for different periodic fiber arrangements (square edge-packing, diagonal-packing and triangle-packing); unit cell with many fibers for random fiber arrangement	Stress-strain responce of and stress distribution in MMC with different fiber arrangements is obtained. It is shown that the effect of fiber distribution on the constitutive response is stronger than that of fiber shape.	6061-O Al alloy reinforced with boron fibers	[20]
Effect of fiber arrangement and clustering on stress fields and damage initiation in composites	ABAQUS. Square unit cell with an off-center fiber	Microscale stress and strain fields are computed for periodic, modified periodic and clustered periodic fiber arrangement	Al reinforced by boron fibers	[7]
Effect of fiber arrangement on microscale stress field and overall response in MMC	ABAQUS. Unit cell approach. Perturbing periodic square array of fibers to model deterministic but less ordered fiber arrangements. Staggered and non-staggered arrangements are modelled by a reference volume consisting of two symmetric subcells.	Overall response 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 0^o direction – periodic hexagonal arrangement - periodic square array in the 45^o direction.	Al reinforced with Altex fibers	[8]
Correlation between parameters of random distribution of fibers on the stress field and crack initiation	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)	Local stress fields are determined for different fiber distributions. It is shown that clustered fibers are most sensitive toward nucleation of cracks	Unidirectional glass composites with long fibers	[21]
Study of deformation and damage in fiber reinforced composites	Axisymmetric unit cell (short and long) with fiber and matrix, which contains cohesive elements (surface elements between other continuum FEs, which can fail)	It is shown that a strong interface leads to high stress concentrations in the fiber; matrix toughness influences strongly the debonding.	Calcium aluminosilicate reinforced with SiC fibers	[34]
Effect of fiber volume fracton and matrix strain hardening parameters on	Self-consistent embedded cell model: circular fiber is surrounded by metal matrix,	Stress-strain curves are obtained for square and hexagonal fiber arrangement	Al with 46 % boron fibers	[13], [14]

the limit flow stress and stress-strain behaviour of composite under transverse loading is investigated	which is in turn embedded in the composite material.	and for different shapes of the embedded cells. Design formula.		

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 behaviour can be studied.

A further development of the unit cell approach is presented by the **unit cell with many inclusions** [20, 21]. 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. Brockenborough et al. [20] used the unit cell with many inclusions to study the behaviour of fiber reinforced composite with random distribution of fibers. Axelsen, and Axelsen and Pyrz [21, 22] have applied the unit cell model to study the effect of parameters of random distribution of fibers on the mechanical properties and damage behaviour 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. Siegmund et al. [23] 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 and have been distributed randomly.

In several works, **combinations** of unit cell models **with other numerical** or analytical **approaches** is used to model the behaviour of material with regularity on only one scale level and without any periodicity on other levels; the behaviour of such a material on different scale levels is simulated with the use of different approaches. Plankensteiner, Böhm, Ramerstorfer and colleagues [7,8,24,25] have developed several hierachical 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 behaviour at other scale levels is described analytically, as layered or gradient material. Hönle et al. [12] and Mishnaevsky Jr et al. [5] have reported also a two-level model of material behaviour: the stress-strain curve was obtained from unit cell model and then assigned to each finte element in the FE model of Al/Si cast alloy; it allowed to model the damage propagation in the alloy.

The generalisation of the 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. Such a cell allows to simulate the material behaviour 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 assumes some porosity [26]. The further development in the 3D unit cell modelling is the use of prismatic and cubic unit cells [27]. The unit cell consisting of many unit axisymmetrical unit cells („super element“) developed in [28, 29] allows to take into account both non-regularity of material structure and 3D effects.

From above consideration and the results of applications of UCA given in Tables 1-4, one can draw a conclusion that the unit cell approach is developing in the following directions:

1. **Taking into account the random structure of material (non-regularities and non-periodicity in the material structure):** from simple two-dimensional round fiber-matrix unit cell (which allowed to study the effect of elastic/plastic constants of filler and matrix, and the volume fraction of filler on the mechanical behaviour of composite; such cells are applicable only to the quantitative analysis of the

behaviour of fiber-reinforced composites or qualitative analysis of the behaviour of particle-reinforced composites) to the unit cell with off-center fiber, then to the unit cells with the inclusion which presents several (also, randomly distributed [Axelsen, Pyrz and Axelsen [21,22]) inclusions with matrix.

2. **Hierarchical models:** 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 [8], "super-elements" [28], etc).
3. **From 2D to 3D:** from simplest axisymmetric cylindrical unit cells with spherical inclusions to prismatic and cubic unit cells [26], "super-elements" from many cylindric unit cells [26, 27], etc.

One may note that the unit cell approach is used mainly to solve the following problems:

- to study the effect of the mutual arrangement of phases on the mechanical behaviour of the composite,
- to clarify the mechanisms of damage initiation, or
- to study the initial stages of void formation and growth (see Table 4).

2.2. Real Structure Simulations

As shown above, the unit cell simulation is applicable and efficient 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 [4, 24, 31,32]: this is correct both for direct real structure calculations and for the approximation of material structure by the unit cell [7].

The FE simulation of the mechanical behaviour of multiphase materials which takes into account the real structure of these materials can be carried out with the use of one of the following numerical approaches:

1. **traditional (single-phase) finite elements**. In this case, different material properties may be assigned only to different to finite element and the phase boundaries must coincide with the edges of finite 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.
2. **multiphase finite elements (MPE)**, developed by Steinkopff and Sautter [33], Sautter [30], Wulf [9], Schmauder et al. [31, 32], etc. The idea of the method of multiphase elements is that the different phase properties are assigned to individual integration points in the element. Therefore, 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. The possibility of using initial meshes of arbitrary simple structures for the simulation of the behaviour of complex materials is the main advantage of the method of multiphase elements. On the other hand, MPE does not allow to take into account fine effects of interfaces.

One of recent results in the simulation of real structures is the development of a 3D multiphase finite element [4, 32]. 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 behaviour of heterogeneous materials taking into account their structure in cases when other methods are hardly applicable.

The real structure simulations, especially the 3D MPE version, 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

Table 2. Simulation of Mechanical Behaviour and Fracture of Particle-Reinforced Composites and Alloys

Problems	Numerical approach and used codes	Main results	Materials considered	Refs.
Analysis of the plastic zone size in front of crack	Various microstructures, obtained from micrographs, was idealized to correspond the FE mesh. "Nodal-tie dislocation elements" were used to model the grain/grain interfaces.	Growth of the plastic zone in front of the crack as a function of the load was studied. 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	WC-Co hard alloys	[35]
Study of the effect of shape, concentration and distribution of particles on the overall elastic responce of composites	Plane strain and axisymmetric unit cell; cylinder, truncated cylinder, double-cone and sphere shapes of reinforcement;	The shape of reinforcements significantly effects the elastic properies of the composites; the forms of inclusions which ensure maximal and minimal Young's moduli of the composites are determined.	Al alloys with SiC reinforcement; Al-Cu alloys; other composites	[36]
Study of plastic deformation of binder in front of a crack	ASKA. Real structure embedded in homogeneous surrounding.	It is shown that ligaments between carbides fail by nucleation and growth of pores at the points where the crack from carbides enters the ligament.	WC-Co hard metals	[37]
Simulation of large plastic deformation of coarse two-phase materials	LARSTRAN. Hexagonal unit cell. Single-phase element and MPE, remeshing (repeated). Akima interpolation. Both fibre and matrix deform plastically.	It is shown that if the spatial distribution of the harder phase is very irregular, strain localization in the softer phase becomes less pronounced. The rotation of fibres during transverse deformation is a result of large plastic deformation in the matrix.	Ag-Ni fiber composite with 58.4 vol. % Ni	[33]
	LARSTRAN. Real structure simulation. MPE; simulation with and without remeshing (repeated). Akima interpolation.		Ag-Ni particle composite (32 vol. % Ni) and Ag-Ni fiber composite (58.4 vol. % Ni)	

Simulation of crack initiation and propagation in real structures of a multiphase material	PATRAN, LARSTRAN. MPE, EET. Real structure of material is reproduced by image analysis of micrographs. RS is embedded in the composite cell.	The numerically determined crack path reproduces very good the experimentally observed crack path	Al (6061) with 20 % SiC particles	[9]
Simulation of crack initiation and propagation in real structures of a multiphase material	PATRAN, LARSTRAN. MPE, EET. Real structure of material is reproduced by image analysis of micrographs. Rice-Tracey damage parameter as a condition of element elimination in matrix and critical maximum stress – in particle.		AlSi7Mg cast alloy (consisting of Al matrix and Si patricles)	[39]
Simulation of deformation of real 3D structures	PATRAN, LARSTRAN. 3D MPE. Image analysis of micrographs of many sections of materials is used to reconstruct 3D real structure	Efficiency and applicability of 3D MPE is verified and proved		[32]
Simulation of deformation in real structures	ABAQUS. Real structure of material is reproduced by image analysis of micrographs with the use of *Verborde* and *Digit* codes. FE meshes from square elements which are automatically associated with correponding material.	Stress-strain curves of two-phase steel are obtained and compared with the stress-strain curves of components. The evolution of stresses and strains during loading is studied.	Duplex steels (ferrite + austenite)	[10]
Analysis of relation between stresses in particles and averaged macrostresses	ABAQUS. Axisymmetric unit cell (with spring elements to control stress triaxiality) consisting of elastic round particle and elasto-plastic matrix	General relation between local stresses in the particle and on continuum level is obtained	AlMgSi alloy	[38]
Effect of contiguity of phases on the plastic flow of two-phase alloys	ABAQUS. Unit cell which consists of an array of hexagons. The hexagons represent grains of two phases, which are randomly distributed.	Limit flow stress of the material is calculated for different volume fractions and contiguities of phases	Model two-phase material with coarse structure	[23]
Effect of particle shapes, orientation and volume fraction on theelastic moduli and stress-strain curves of MMC	3D hexagonal and cubic unit cell with spherical, cylindrical, cubic and rectangular particles with varying orientations.	The higher an aspect ratio of particles in a given direction, the more effective reinforcement in that direction.	Al alloy (Al 2024-T851) with Al_2O_3 particles.	[74]
Effect of non-metallic particles on deformation and shear band formation	PATRAN, LARSTRAN.MPE. Real and artificial microstructures with different particle arrangement (random, strong and weak stripes, etc)	The more localized the particles in the stripes, the stronger the stress concentration in shear bands. Sites of possible microcrack initiation are determined.	Al (6061) reinforced with 10 % SiC-particles arranged in stripes with clusters and gaps inside	[40], [41]
Effect of shapes, volume ratio,	Two-level model: 1) Axisymmetric (cylindrical) unit cell model with	Stress-strain relationships for alloys with different particle	Al alloys with SiC particles	[28], [29]

mutual interaction of particles and their spatial distribution on damage formation and strength of MMC	elliptical particle; model with and without constraints. 2) Box-shaped super element: model consisting of many unit cells with different particle volume fraction and shapes.	aspect ratio, volume fraction, availability and non-availability of side constraints, uniform and non-uniform particle distribution are obtained. Damage initiation in matrix and debonding are studied for different particle distributions.		

studying the real materials) is possible only with some tricks, real structure simulations allow the analysis of the effect of material structure on properties without any principal limitations.

3. Modelling of the Mechanical Behaviour of Structural Materials

Tables 1-3 give methods used, considered problems and some results in the area of the modelling of the behaviour of fiber-reinforced and particle-reinforced composites, steels and alloys.

Fiber-reinforced composites (FRC) under transverse loading present the simplest object of the numerical simulation of the material behaviour taking into account its structure: in this case, one may assume that a two-dimensional problem is solved. Therefore, all classical methods of computational mesomechanics of materials, including real structure simulation, have been initially developed for or tested on fiber-reinforced composites.

One can see from Table 1 that the problems which are considered in modelling composite behaviour most often are the effect of the distribution of fibers on the strength, stress state in the composites or stress strain behaviour. In some cases, the damage mechanisms in these composites are studied as well. All problems are solved with the use of the unit cell approach which fits ideally for the simulation of the behaviour of FRC under transverse loading.

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. So, such materials can be modelled by means of the periodic microfield approach only with some losses of information about the structures. That is why real structure simulations play an especially important role in the simulation of the mechanical behaviour and failure of steels. Another way to avoid such difficulties is the hierarchical approach developed by Rammerstorfer and colleagues [24, 25]. Some investigations of the mechanical behaviour of steels and alloys are given in Tables 2 and 3.

4. Damage and Fracture

The fracture process in heterogeneous materials consist normally on several stages: formation of voids and microcracks in random sites throughouth 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 [46]. All of these stages are strongly influenced by the inclusions and voids available in the material.

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 considered). The micromechanical modelling 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 disrepancies between quasi-continuum statement of a problem in the framework of FEM and random, discontinuous nature of crack growth.

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 consider only some aspects of this problem. Let us look at 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.

4.1. Initiation and Growth of Voids

To model the initiation and growth of voids in materials, the **unit cell approach** (UCA) is used

Table 3. Simulation of Strength and Fracture Behaviour of Steels

Problems	**Numerical approach and used codes**	**Main results**	**Materials considered**	**Refs.**
Deformation and the onset of damage formation				
Overall response of steels as well as mechanisms of local failure in steels with real structures are studied. The effect of progressive carbide cleavage on the stress-strain curve is considered.	PATRAN, ABAQUS. Mesophase Cell . Hierarchical Modelling: mesoscale unit cell model, which is constructed on the basis of image analysis of steel micrographs and statistical averaging of properties at microlevel; transformation field approach or incremental Mori-Tanaka approach.	Stress-strain curves, and distributions of maximum principal inclusion stresses are obtained. It is shown that the carbide grain cleavage is a main fracture mode at the microscale.	Electroslag remelted HSS, with netlike carbide arrangement	[24]
Stress distribution, and also an effect of initial thermal residual stresses on the parameters of stress distribution are considered.	HEXGRAIN, ABAQUS. Hexagonal Cell Tiling (HCT) Concept: unit hexagonal cells containing a number of inclusions.	Stress level within carbide particles, and in the matrix, and the effect of thermal stresses on them are studied.		

Overall response of steels as well as mechanisms of damage in steels with real structures are studied	"Micro-Meso-Macro Model": Each carbide stringer is treated as particle reinforced matrix-inclusion composite with the use of statistical averaging technique (multi-particle effective field method [25]); at mesolevel, HSS is modelled as laminated composite.	Distributions of maximum principal and interface stresses are obtained	Electroslag remelted HSS, with layered carbide arrangement	[25]
	HCT Concept: 2D unit cell with a number of inclusions at microlevel; at mesolevel, HSS is treated as MMC with a compositional gradient	As above	As above	[25]
		Distributions of maximum principal stresses in the matrix are obtained		
Stress distribution in the vicinity of hard inclusions or voids in soft matrix; simulation of deformation of coarse two-phase materials	FINEL (elasto-plastic and rigid-plastic); Local refinement of FE mesh in the vicinity of hard inclusions, or in the region of a material element (an element with real structure, which was embedded in homogeneous material with coarse FE mesh)	Effect of relationships between mechanical properties of inclusion and matrix on local stress concentration, and deformation in real structure are studied.	Stahl St37; Model material	[42]
Crack initiation and propagation				
Influence of carbide particle distribution on the fracture processes in steel is investigated.	CRACKAN. Modelling of real structures. Plasticity of matrix is modelled with J_2 flow theory. Carbide particles fail due to cleavage along crystallographic planes.	Stress distribution in real microstructure ahead of main crack, local damage and effect of local triaxiality on clevage strength of carbides are studied.	Ledeburitic chromium steel SAE-D3 in as cast condition and hot worked state	[11]
Simulation of crack initiation (also in front of main crack) due to the particle cracking and interfacial failure	CRACKAN (like above). Decohesion between carbides and matrix occurs if the stresses normal to the interface reach a critical value. Unit cell model is used to study the interaction between inclusions.	Particle cracking, damage evolution in front of main crack are studied.	Ledeburitic chromium steel SAE-D with different states of heat treatment; HSS manufactured by powder metallurgy and HIP	[43]

Crack initiation by carbide failure is simulated	ANSYS. Crack faces are predefined with the use of non-linear spring elements	Crack distribution in real structure of steel. It is shown that long and thin carbides fail primarily and form initial cracks.	Electroslag remelted HSS, with 50 % hot reduction	[45]
Stress and crack distribution in real structures is obtained; effect of carbide stringer width of the crack formation is studied.	LARSTRAN. Method of multiphase elements (MPE) makes possible to simplify preprocessing and variation of carbide stringer width. Automatic element elimination technique is used to model crack initiation and growth.	Crack initiation, growth and distribution in real structure of HSS	Electroslag remelted HSS, with 50 % and 97.7 % hot reduction	

widely. Some models based on this approach are given in Table 4. One can see from Table 4 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 behaviour of the material (i.e. stiffness reduction); simulation of particle failure, interface cracking and their effect on the stiffness of material.

It is clear that the use of the unit cell approach in modelling 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 overcome with the use of the embedded unit cell [13]; in this case, the effect of other voids can be taken into account through the boundary conditions and the properties of embedding.

4.2. 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 [54, 55] , and then, the crack propagation.

Generally, there are two main approaches to the numerical simulation of fracture: a crack can be modelled as a discontinuity between adjacent elements, and a crack may be „smeared“ over entire elements [56, 57]. 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 [57]; the smeared crack model does not exclude the stress transfer across a widely open crack in some cases [57]. 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 [61, 62] 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 [63], or triangular or brick elements with an interpolation function, which contains an inverse square root of the singular stresses [61. 62]; these elements are located at the crack front. As conditions of crack growth, strength or fracture based criteria [56], or damage parameters (like the Gurson-Tvergaard-Needleman model for void growth model in ductile materials [64], or continuum damage models by Krajcinovic and Fonseka for brittle materials [65]) 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 modelling fracture in materials.

In the **cohesive zone models** (CZM) [66] 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 [67]. Yet, by introducing the so-called length scale parameters into the formulation the dependence of the solution on the element size can be eliminated [67]. Siegmund et al. [64] have considered interrelations between the model of crack growth based on the void evolution and coalescence (modelled with the Gurson-Tvergaard-Needleman approach) and CZM, and developed a version of CZM which takes into account the local stress triaxiality in front of crack.

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 neighbouring 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 neighbouring 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 [31]. The main advantages of this approach are that both microdamage and crack propagation can be simulated, and that the damage evolution in multiphase materials can be efficiently described.

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" [68].

The **computational cell methodology** (CCM), developed by Xia and Shih [69]-[71] 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 [72] 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 main idea of the **cohesive surface model** (CSM), developed by Mintchev [67], is that a criterion for decohesion 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.The difference between this model and the cohesive zone is that the decohesion criterion is not comprised as a constitutive law of a thin material layer joining the two parts of the system. CSM is used with the FE code ABAQUS [67],

The **hybrid fracture/damage approach** (HFDA) suggested by van Vroonhoven and Horsten [62] seeks to combine some idea 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) in order to avoid the disadvantages of both approaches (necessarity of frequent adaptation of FE mesh for fracture mechanics model, and mesh and damage localization sensitivity in the damage-based models). In the framework of this approach, a so-caled "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

Table 4. Simulation of Void Initiation and Evolution

Problems	**Numerical approach and used codes**	**Main results**	**Materials considered**	**Refs.**
Study of the effect of cracks in particles and interfacial debonding on the strength and creep resistance of composites	ABAQUS. 1) Three phase damage cell model (hexagonal unit cell with fractured particle; the crack plane is perpendiculat to the direction of stressing; the cel is transformed into axisymmetric one), embedded into composite with undamaged particles. 2) Modification of above 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 behaviour is studied.	MMC (Al, Ti and Ni alloys reinforced with Al_2O_3)	[47]
Study of effect of void nucleation in matrix on the deformation of composites	Axisymmetric cylindrical unit cell with reinforcement of different shapes (cylinders, whiskers and spheres). Constitutive behaviour of matrix is given by Gurson model.	Overall stress-strain responce for MMC with different reinforcement, and distributions of void volume fraction, stress and strain distribution in matrix are obtained. It is shown that the factors which increase the constraints on plastic flow (like hydrostatic stress), tend to decrease the overall strain to matrix failure.	Al alloys with particulate and whisker SiC reinforcement	[48]
Effect of reinforcement clustering on the deformation of composites	Unit cell with different arangements of inclusions. Gurson model for matrix behaviour.			
Simulation of initiation and growth of spherical voids in elasto-plastic metals	ABAQUS. Modified Riks method is used to solve the instability problems. Cylidrical unit cell.	Effect of parameters of multiaxiality on the elasto-plastic behaviour of material, local stresses, void volume and its critical level is studied	Model material	[49]

Influence of stress triaxiality and void shape on the critical void volume	ABAQUS. Cylindrical unit cell	Effective stress vs. Strain curves and void volume fraction vs. strain curve are obtained; the parameters of Gurson-Tvergaard-Needlemen model are determined from cell calculations.	Ferritic nodular iron GGG-40 with different graphite morphology	[50]
Influence of spatial void arrangement and stress triaxiality on damage processes	ABAQUS. 3D hexagonal and cubic unit cell	The possibility of modelling of graphite nodules by voids is considered; it is shown that the spatial arrangement of periodic arrays of voids influences the deformation behaviour only weakly, but affects strongly the plastic collapse	Nodular cast iron	[26], [27]
Analysis of void growth (up to a state near the occurence of void coalescence) in a thin ductile layer between ceramics	Axisymmetric unit cell with spherical void in the center of cell. Remeshing procedure is used.	The traction-separation law which describes the crack growth by ductile mechanism is determined	Ceramic with thin metall layers	[51]
Effect of distribution of microcracks on constitutive response of creeping solids	3D hexagonal cells and tetrakaidekahedrons (b.c.c. cells) from power-law creeping material with penny-shaped cracks	Constitutive responses of the material at different microcrack densities and stress states are studied	12% Cr ferritic steels	[52]
Study of mechanical behaviour of particle-filled composites when the separation of matrix from filler takes place	Unit cell model (cylinder matrix cell with rigid spherical inclusion). Large deformation approach.	Ultimate strength of composites is determined, and its dependence of the filler content is analyzed. Effective moduls vs. filler concentration curves are obtained.	Elastomeric, particle filled composites with filler content up to 67 %	[18], [19]
Effect of particle cracking and particle debonding on void growth in matrix	Axisymmetric unit cell with ellipsoidal, broken or debonded particle	Stress-strain curves are obtained for different particle shapes and broken or debonded particles	Al with 21.3 % SiC particles	[16]
Effect of biaxial and multiaxial load on damage growth	ADINA. Unit cell with perfectly bonded and perfectly debonded (being simulated as contact surface) interface	It is shown that the interfacial layer is more easily damaged under biaxial than under uniaxial loading.	Al with 10 % Al_2O_3 inclusions	[17]
Simulation of crack	Axisymmetric cylindrical unit cell	The dissipation of energy	Model material	[53]

propagation by void growth and coalescence ahead of a crack tip	from a rigid-perfectly plastic material, with a spherical void; the size of void as related to the radius of the cell is varied. Velocity field is analyzed.	during void growth per unit of fracture surface is shown to be proportional to the distance between voids.		

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 dynamicaly). 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.

One can see that the HDF Approach, 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 considered 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 concretes is given in [59]. In the smeared crack models [58], 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 distancce 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 [60],], 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 [57] seeks to combine strong points of both discrete and smeared approaches to the crack modelling 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 behaviour is taken into account not at the level of FE model, but at the level of the formulation of the method.

4.3 FE-Simulation of Damage and Fracture: Some Comments

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 furtherly 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 [53][64]) or relating these two concepts [67]) 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 modelling.
- 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 [64], [67] or by considering mesh size "as an independent parameter in the local approach to fracture" [68], this problem remains to be a basical problem of mesomechanical modelling of failure of materials.

- In several widely accepted approaches (CCM. CZM. CSM), the **crack path** has to be **prescribed**; this presents an additional strong assumption which makes it impossible to analyse 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 modelling 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 [76, 77], EET and MPE model –[4, 9], and also numerical methods based on construction of pseudodifferential operators of the crack equilibrium problem [78, 79]).
- 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 discontinuitis 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.

5. 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.
Let us look firtstly 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 brocken particles, or with several particles),
- hierarchical or many-level modelling [5, 24, 25], super element [28] or layered or network-like combinations from unit cells [24,25], unit cell with embedding or, reversely, inclusion, which have properties, averaged over some volume of material or some amount of inclusions [21], 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 behaviour of materials without any observable regularity of structure or with structure irregularities which determine the material behaviour 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 **multi-level simulation** or **hierarchical modelling**, which was mentioned above in connection with the tendences 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 behaviour (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) [80] and the **crystal plasticity modelling** (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 behaviour) [81, 82].

As can be seen from the above analysis of the simulation of damage and fracture, the processes can be modelled 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 developed in [17]).

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 [58]. 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 – see Figure 1. 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.

Some Abbreviations:

BE	-	boundary element
CCM	-	computational cell methodology
CSM	-	cohesive surface 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

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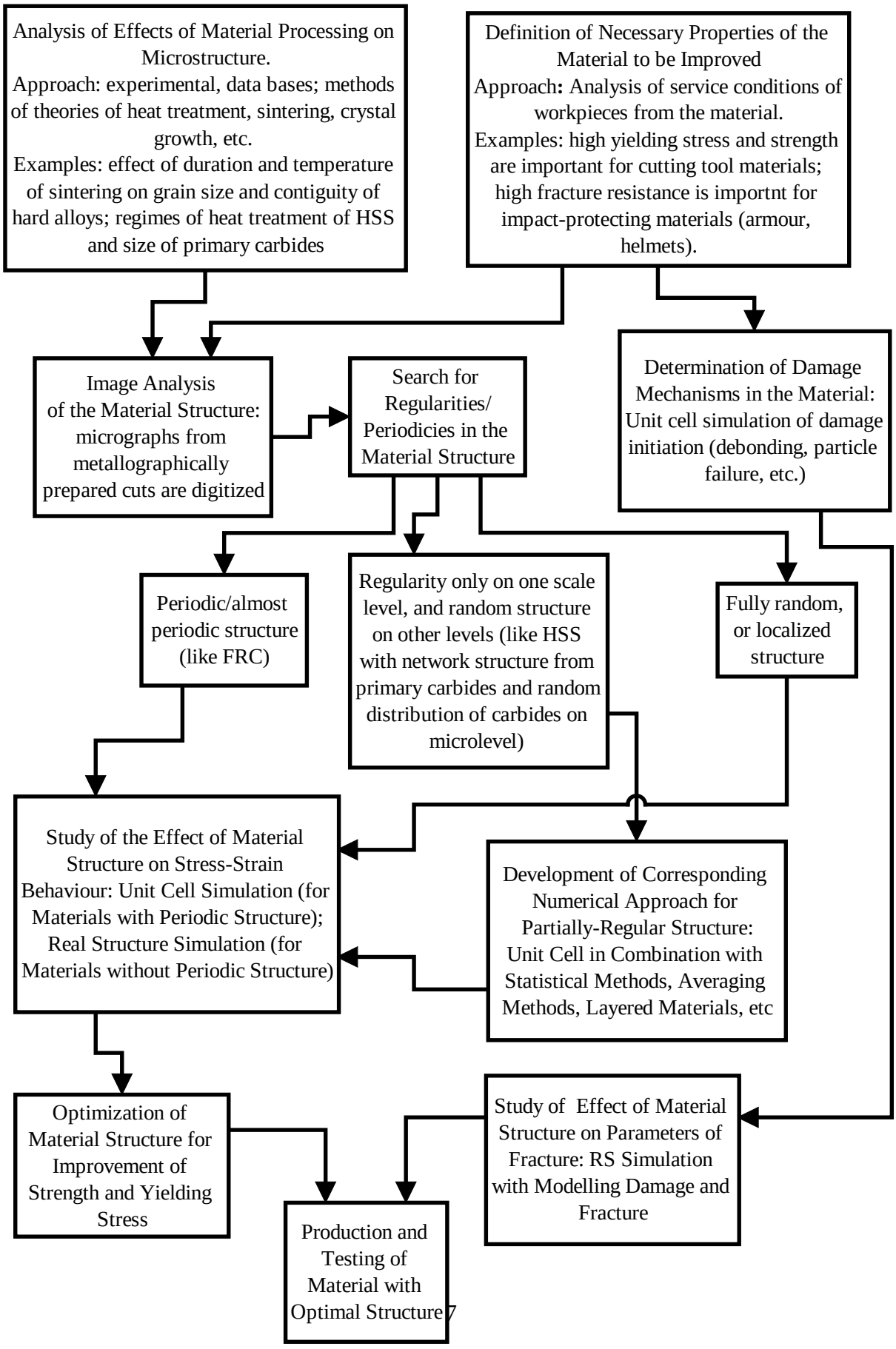

Figure 1. Improvement/Design of Materials on the Basis of Computational Micro- and Mesomechanics