

Chapter 2: Micromechanical Simulation of Composites

The microstructure (fixed by features such as the grain size, the presence of particles, layers/coatings, impurities, and internal interfaces) frequently determines the properties (such as strength, toughness, and fracture energy) of advanced materials. Because the microstructure is determined during production (by parameters such as temperature, time, and pressure) and the properties are determined in application (e.g., implementation and life-time), the microstructure/property-relationship (Figure 2.1) has been the focus of many investigations in the recent past. This relationship especially requires knowledge of how to link the different length scales in modeling and characterizing these materials.

The linkage of modeling on the nanoscale (nm-length scale) with that on the macroscale (length scale of real specimens) is a current challenge in materials science. Despite cheaper and faster computer resources, it is still difficult to inflate atomistic models of crystals to the size of specimens and components. Special problems of crack propagation have been successfully treated by dedicated coupled atomistic continuum methods [1, 2]. Nevertheless, a general method to connect theoretical calculations on the nanoscale with the macroscale is not available. Instead, at present it seems more promising to restrict oneself to selected materials problems and to connect different length scales by qualified physical laws that describe corresponding materials behavior [3, 4]. The terminology of relevant length scales, together with referring physical phenomena and methods, is illustrated in Figure 2.2 [5]. These methods require knowledge on the atomistic level.

examples of fiber and particulate-reinforced composites. It should be noted that when continuum mechanical methods are applied, the relevant microstructural features such as particle sizes or phase areas have to be large enough (in the micrometer regime or above) in order to be modeled appropriately.

In section 2.1, the limit flow stresses for transverse loading of metal matrix composites reinforced with continuous fibers and for uniaxial loading of spherical particle reinforced metal matrix composites are investigated with the use of embedded cell models. A fiber of circular cross section or a spherical particle is surrounded by a metal matrix, which is again embedded in the composite material with the mechanical behavior to be determined iteratively in a self-consistent manner. Stress-strain curves have been calculated for a number of metal matrix composites with the embedded cell method and compared with literature data of a particle reinforced Ag-58vol.%Ni composite and for a transversely loaded uniaxially fiber reinforced Al-46vol.%B composite. Good agreement has been obtained between experiment and calculation and the embedded cell model is thus found to represent well metal matrix composites with randomly arranged inclusions.

Systematic studies of the mechanical behavior of fiber and particle reinforced composites with plane strain and axisymmetric embedded cell models are carried out to determine the influence of fiber or particle volume fraction and matrix strain-hardening ability on composite strengthening levels. Results for random inclusion arrangements obtained with self-consistent embedded cell models are compared with strengthening levels for regular inclusion arrangements from conventional unit cell models. It is found that with increasing inclusion volume fractions there exist pronounced differences in composite strengthening between all models.

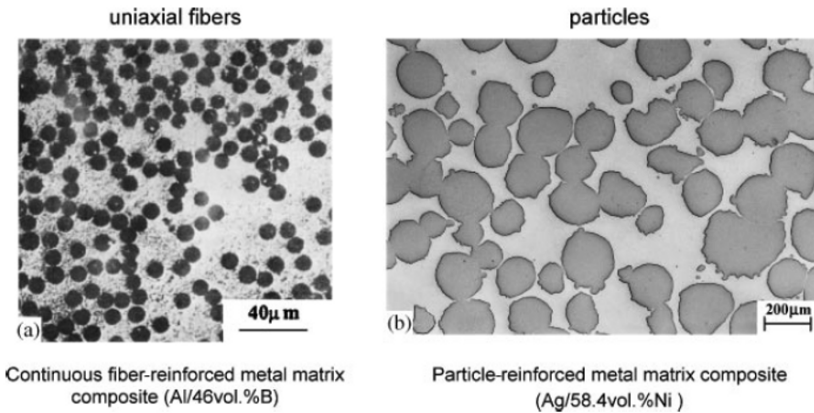


Fig 2.3 Typical microstructures to be modelled in computational mechanics. (a) Al/B_f fiber-reinforced MMC, (b) Ag/58.4vol.%Ni particle-reinforced MMC.

Finally, closed-form expressions are derived to predict composite strengthening levels for regular and random fiber or particle arrangements as a function of matrix hardening and particle volume fraction. The impact of the results on effectively designing technically relevant metal matrix composites reinforced by randomly arranged strong inclusions is emphasized.

In section 2.2, the 3D-multiphase finite element approach is presented. This approach permits finite-element-modelling of the plastic deformation of realistic 3D-microstructures. In contrast to conventional ‘single phase elements’ where the phase boundaries are simulated by element edges, the ‘multiphase element’ can be assigned to different materials when a phase boundary runs across it. The 3D-multiphase element is firstly applied to a simple test geometry. The efficiency of the 3D-multiphase element method is demonstrated by the analysis of a more complex 3D-microstructure. Finally, for a comparison of 2D- and 3D-simulations the stress distribution obtained in the 3D-calculation is compared with the results of a 2D-simulation of a representative intersection of the microstructure.

In section 3.3, different methods of automatic generation of 3D microstructural models of materials are discussed. A program for the automatic generation and the design of FE meshes for idealized 3D multiparticle unit cells (with spherical inclusions) is presented. Numerical testing of Al/SiC composites with random, regular, clustered and gradient arrangements of spherical particles is carried out. The fraction of failed particles and the tensile stress-strain curves were determined numerically for each of the microstructures. It is found that the strain hardening coefficient increases with varying the particle arrangement in the following order: gradient < random < clustered < regular microstructure. The variations of the particle sizes causes strong decrease in the strain hardening rate of the composite, and leads to a quicker and earlier damage growth in the composites.

Further, another approach to generate 3D FE models of composites based on the procedure of a step-by-step packing (SSP) of a finite volume with structural elements is discussed. This has been used to design the composite structure consisting of an Al(6061)-matrix with Al_2O_3 -inclusions. A three-dimensional mechanical problem of the structure behaviour under tension has been solved numerically, using both an implicit finite-element method and an explicit finite-difference code. Special attention is given to the comparison of quasi-static and dynamic calculations. Evolution of plastic deformation in the matrix during tensile loading has been investigated. Qualitative and quantitative analysis of different components of stress and strain tensors is provided on the basis of mesomechanical concepts. Based on 3D-analyses, the conclusions regarding the approximations when considering deformation behaviour on meso and macro scale levels have been performed.

Finally in this chapter, yet another method for the reconstruction and generation of 3D microstructures of composites based on the voxel array data is presented. The geometry-based and voxel array based methods of reconstruction and generation of finite element models of 3D microstructures of composite materials are discussed and compared. With the use of the developed program, the deformation and damage evolution in composites with random and graded microstructures were numerically simulated. The tensile stress-strain curves, fraction of failed

elements, and stress, strain and damage distributions at different stages of loading were determined for different random microstructures of the composites. It is shown that the stiffness, peak and yield stresses of a graded composite decrease with increasing the sharpness of the transition zone between the region of high volume content of the hard phase and the reinforcement free region. The critical applied strain, at which the intensive damage growth begins, is decreasing with increasing the volume content of the hard phase of the composite.

References

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2.1 Embedded unit cells¹

Metal matrix composites (MMCs) are defined as ductile matrix materials reinforced by brittle fibers or particles. Under external loading conditions the overall response of MMCs is elastic-plastic. MMCs are frequently reinforced by continuous fibers which are aligned in order to make use of the high axial fiber strength. However, the mechanical behavior of these composites under transverse loading is well behind their axial performance [1-7]. On the other hand, it is well known, both from experiment and calculations [8] that details of transverse strengthening in uniaxially fiber reinforced MMCs are a strong function of fiber arrangement. To derive the mechanical behavior of MMCs, a micromechanical approach is usually employed using cell models, representing regular inclusion arrangements. As regular fiber spacings are difficult to achieve in practice, most of the present fiber reinforced MMCs contain aligned but randomly arranged continuous fibers. Thus, the accurate modeling of the mechanical behavior of actual MMCs is very complicated in practice even if the fibers are aligned.

Initially, the transverse mechanical behavior of a unidirectionally continuous fiber-reinforced composite (A1-B) with fibers of circular cross section was studied by Adams [9] adopting finite element cell models under plane strain conditions: a simple geometrical cell composed of matrix and inclusion material is repeated by appropriate boundary conditions to represent a composite with a periodic microstructure. Good agreement was achieved between calculated and experimental stress-strain curves for a rectangular fiber arrangement. The influence of different regular fiber arrangements on the strength of transversely loaded boron fiber reinforced Al was analyzed in Refs [2, 5, 7]. It was found that the same square arrangement of fibers represents two extremes of strengthening: high strength levels are achieved if the composite is loaded in a 0° direction to nearest neighbors while the 45° loading direction is found to be very weak for the same fiber arrangement. A regular hexagonal fiber arrangement lies somewhere between these limits [2, 5, 7, 10, 11]. The transverse mechanical behavior of a realistic fiber reinforced composite containing about 30 randomly arranged fibers was found to be best described but significantly underestimated by the hexagonal fiber model [5]. One reason for the superiority of the hexagonal over the square arrangement in describing random fiber arrangements is due to the fact that the elastic stress invariants of the square arrangement agree only to first order with the invariants of the transversely isotropic material while the hexagonal arrangement agrees up to the second order [10]. Dietrich [6] found a transversely isotropic square fiber reinforced Ag-Ni composite material using fibers of different diameters. A systematic study in which the fiber volume fraction and the fiber arrangement effects have been investigated was founded into a simple model in Ref. [11].

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The influence of fiber shape and clustering was numerically examined in some detail by Llorca *et al.* [12], Dietrich [6] and Sautter [13]. It was observed that faceted fiber cross sections lead to higher strengths compared to circular cross sections except for such fibers which possess predominantly facets oriented at 45° with respect to the loading axis in close agreement with findings in particle reinforced MMCs [14]. Thus, hindering of shear band formation within the matrix was found to be responsible for strengthening with respect to fiber arrangement and fiber shape [12]. In Refs [8, 11, 15, 16] local distributions of stresses and strains within the microstructure have also been identified to be strongly influenced by the arrangement of fibers. However, no agreement was found between the mechanical behavior of composites based on cell models with differently arranged fibers and experiments with randomly arranged fibers loaded in the transverse direction.

The overall mechanical behavior of a particle reinforced composite was studied with axisymmetric finite element cell models by Bao *et al.* [17] to represent a uniform particle distribution within an elastic-plastic matrix. Tvergaard [18] introduced a modified cylindrical unit cell containing one half of a single fiber to model the axial performance of a periodic square arrangement of staggered short fibers. Horn [19] and Weissenbek [20] used three dimensional finite elements to model different regular arrangements of short fibers and spherical as well as cylindrical particles with relatively small volume fractions ($f < 0.2$). It was generally found that the arrangement of fibers strongly influences the different overall behavior of the composites. When short fibers are arranged in a side-by-side manner, they constrain the plastic flow in the matrix and the computed stress-strain response of the composite in the fiber direction is stiffer than observed in experiments. If the fibers in the model are overlapping, strong plastic shearing can develop in the ligament between neighboring fibers and the predicted load carrying capacity of the composite is closer to the experimental measurements. In Ref. [21] the stress-strain curves based on FE-numerical solutions of axisymmetric unit cell models of MMCs are given in a closed form as a function of the most important control parameters, namely, volume fraction, aspect ratio and shape (cylindrical or spherical) of the reinforcement as well as the matrix hardening parameter.

One reason for the discrepancy between experiments and calculations based on simple cell models in the case of particle, whisker and fiber reinforced metals is believed to be the un-natural constraint governing the matrix material between inclusion and simulation cell border [5, 15, 17-19, 22-24] resulting in an unrealistic strength increase. The influence of thermal residual stresses in fiber reinforced MMCs under transverse tension was studied in Ref. [7] and found to lead to significant strengthening elevations in contrast to findings in particulate reinforced MMCs where strength reductions were calculated [25].

A limited study on the overall limit flow stress for composites with randomly oriented disk- or needleshaped particles arranged in a packet-like morphology is reported by Bao *et al.* [17]. In Refs [26, 27] a modified Oldroyd model has been proposed to investigate analytically-numerically the overall behavior of MMCs with randomly arranged brittle particles. Duva [28] introduced an analytical model to represent a random distribution of non-interacting rigid spherical particles

perfectly bonded in a power law matrix. The Duva model is a self-consistent model and should be valid particularly in the dilute regime of volume fractions, $f < 0.2$.

In this work, cell models are applied to simulate, for a number of relevant parameters, the transverse behavior of MMCs containing fibers in a regular square or hexagonal arrangement as well as the mechanical behavior of MMCs containing particles in a regular arrangement. MMCs with randomly arranged inclusions are modeled by a recently introduced self-consistent procedure with embedded cell models. This method of surrounding a simulation cell by additional “equivalent composite material” was introduced in Ref. [6] for structures which are periodical in the loading direction and was recently extended to non-periodic two-dimensional [29-31] and three-dimensional composites [13, 27]. The method is known to remove the above described unrealistic constraints of cell models. An initial comparison of two- and three-dimensional embedded cell models in the case of perfectly-plastic matrix material depicts elevated strength levels for the three-dimensional case [27], similar to composites with regularly arranged fibers [11].

The purpose of the present paper is to investigate the mechanical behavior of MMCs reinforced with regular or random arranged continuous fibers under transverse loading, as well as the mechanical behavior of MMCs reinforced with regular or random arranged particles under uniaxial loading, and to systematically study composite strengthening as a function of inclusion volume fraction and matrix hardening ability. The finite element method (FEM) is employed within the framework of continuum mechanics to carry out the calculations.

2.1.1 Model Formulation

A continuum mechanics approach is used to model the composite behavior. The inclusion behaves elastically in all cases considered here and its stiffness is much higher than that of the matrix, so that the inclusion can be regarded as being rigid. In addition, the continuous fibers of circular cross section and spherical particles are assumed to be well bonded to the matrix so that debonding or sliding at the inclusion-matrix interface is not permitted. The uniaxial matrix stress-strain behavior is described by a Ramberg-Osgood type of power law

$$\begin{aligned} \sigma &= E\varepsilon & \varepsilon &\leq \varepsilon_0 \\ \sigma &= \sigma_0 \left[\frac{\varepsilon}{\varepsilon_0} \right]^n & \varepsilon &> \varepsilon_0 \end{aligned} \quad (2.1)$$

where σ and ε are the uniaxial stress and strain of the matrix, respectively, σ_0 is the tensile flow stress, the matrix yield strain is given as $\varepsilon_0 = \sigma_0/E$, E is Young's modulus, and $N = 1/n$ is the strain hardening exponent. Thus, $N = 0$ corresponds to a non-hardening matrix.

J_2 flow theory of plasticity with isotropic hardening is employed with a von Mises yield criterion to characterize the rate-independent matrix material. The von Mises equivalent stress and strain are given as:

$$\begin{aligned}\sigma_v &= \sqrt{3J_2} = \sqrt{\frac{3}{2}s_{ij}s_{ij}} \\ \varepsilon_v &= \frac{1}{1+\nu} \sqrt{\frac{3}{2}e_{ij}e_{ij}}\end{aligned}\quad (2.2)$$

where $s_{ij} = \sigma_{ij} - \sigma_{kk}/3$, $e_{ij} = \varepsilon_{ij} - \varepsilon_{kk}/3$ and ν is Poisson's ratio. In the analytical approach, the metal matrix is considered incompressible, so Poisson's ratio of the matrix will become 0.5 after reaching the yield stress. However, in reality Poisson's ratio of the composite remains below 0.5 as the matrix starts yielding. It changes from the elastic value ν to the limit value 0.5 with increasing yielding zone in the matrix.

The Ramberg-Osgood type of matrix power law hardening is assumed to be valid for the matrix described in terms of von Mises equivalent stress and strain

$$\sigma_v = \sigma_{v0} \left[\frac{\varepsilon_v}{\varepsilon_{v0}} \right]^N \quad (2.3)$$

with the following relations between stress and strain under uniaxial loading and von Mises equivalent stress and strain.

(a) In the case of a two-dimensional (2D) plane strain condition for continuous fiber reinforced composites ($\sqrt{3}/2 \approx 0.866$, $2/\sqrt{3} \approx 1.1547$)

$$\begin{aligned}\sigma &= \frac{\sqrt{3}}{2} \sigma_v \quad \text{with} \quad \sigma_0 = \frac{\sqrt{3}}{2} \sigma_{v0} \\ \varepsilon &= \frac{2}{\sqrt{3}} \varepsilon_v \quad \text{with} \quad \varepsilon_0 = \frac{2}{\sqrt{3}} \varepsilon_{v0}\end{aligned}\quad (2.4)$$

(b) In the case of three-dimensional (3D) axisymmetrical condition for particle reinforced composites

$$\begin{aligned}\sigma &= \sigma_v \quad \text{with} \quad \sigma_0 = \sigma_{v0} \\ \varepsilon &= \varepsilon_v \quad \text{with} \quad \varepsilon_0 = \varepsilon_{v0}\end{aligned}\quad (2.5)$$

The global mechanical response of the composite under external loading is characterized by the overall stress $\bar{\sigma}$ as a function of the overall strain $\bar{\varepsilon}$. Moreover, to

describe the results in a consistent way, the reference axial yield stress σ_0 and yield strain ϵ_0 of the matrix, as defined in equation (2.4) for the 2D case and in equation (2.5) for the 3D case, will be taken to normalize the overall stress and strain of the composite, respectively.

Following Bao *et al.* [17] the composite containing hard inclusions will necessarily harden with the same strain hardening exponent, N , as the matrix for the case of hard inclusions, when strains are in the regime of fully developed plastic flow. At sufficiently large strains the composite behavior is then described by

$$\bar{\sigma} = \bar{\sigma}_N \left[\frac{\bar{\epsilon}}{\epsilon_0} \right]^N \quad (2.6)$$

where $\bar{\sigma}_N$ is called the asymptotic reference stress of the composite which can be determined by normalizing the composite stress by the stress in the matrix at the same overall strain $\bar{\epsilon}$ [equation (2.2)], as indicated in Fig. 2.4:

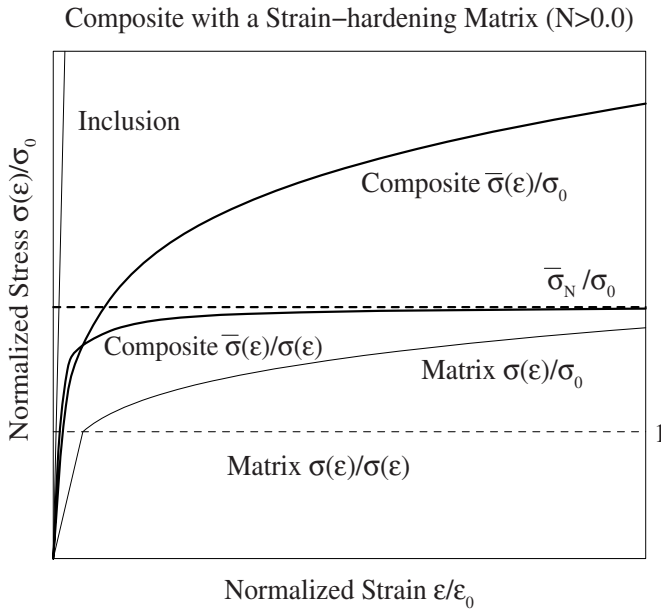


Fig 2.4 Composite strengthening.

$$\sigma_N = \sigma_0 \left[\frac{\bar{\sigma}(\bar{\epsilon})}{\sigma(\bar{\epsilon})} \right] \quad \text{for } \bar{\epsilon} \gg \epsilon_0 \quad (2.7)$$

For a matrix of strain hardening capability N , the limit value $\bar{\sigma}_N / \sigma_0$ is defined as the composite strengthening level, which is an important value to describe the mechanical behavior of composites and which depends only on fiber and particle arrangement, inclusion volume fraction and matrix strain-hardening exponent.

Unit cell models

Before introducing the self-consistent embedded cell model, two regular aligned continuous fiber arrangements, namely square and hexagonal arrangements, and two regular particle arrangements, namely primitive cubic and hexagonal arrangements, are at first considered, as shown in Figs 2.20(a)-(d).

It is well known that the repeating unit cells 1 (or 3) and 2 in Fig. 2.20(a) can be extracted from the regular array of uniform continuous fibers to model exactly the composite with square fiber arrangement under 0° and 45° transverse loading, respectively, whereas the repeating unit cells 6 and 7 (or 8) can be taken from Fig. 2.20(b) to model exactly a hexagonal fiber arrangement under 0° and 30° transverse loading, respectively, if the appropriate boundary conditions are introduced making use of the symmetry conditions. Moreover, the unit cells 4, 9 and 10 can also represent geometrically regular arrangements.

For further simplification the modified unit cells 5, 11 and 12 (circular and elliptically shaped cell models) may be derived from the cells 3, 4, 8, 9 and 10. An ellipsoidal unit cell has been used previously in Ref. [32] and shown to possess very complicated boundary conditions. As can be seen later these unit cells can be employed, however, in the embedding method to model the mechanical behavior of composites with random fiber arrangement.

The results of the unit cell models (as illustrated in Fig. 2.10(b) as an example for three different regular fiber arrangements with non-hardening matrix) show that the composite strengthening levels are quite different, especially at high volume fractions of fibers, with the composite strengthening for square arrangements under 0° loading being highest and for square arrangements under 45° loading being lowest. Further results regarding these three different regular fiber arrangements using unit cell models are given in Ref. [11]. A comparison of the stress-strain curves for the composite Al 46 vol.% B [in Fig. 2.8(a)] shows that the stress-strain curve from random fiber packing given in Ref. [5] lies between the curves from square unit cell modeling under 0° loading and hexagonal unit cell modeling. The curves from square unit cell modeling under 45° loading are even lower. As mentioned above, the strength of composites with randomly arranged inclusions cannot be described by modeling regular inclusion arrangements.

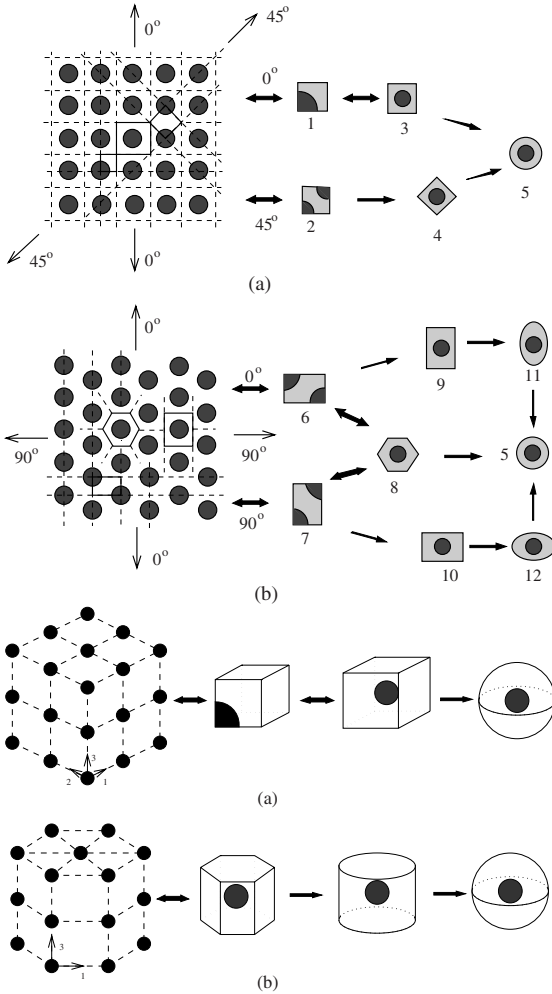


Fig 2.5 Modeling of unidirectional continuously fiber reinforced composites with: (a) square and (b) hexagonal fiber arrangements under transverse loading conditions and particle reinforced composites with: (c) primitive cubic and (d) hexagonal particle arrangements.

Rather, a new model must be employed, which describes approximately the geometry and the mechanical behavior of real composites with randomly arranged inclusions, if models with many inclusions have to be avoided for modeling and computational reasons. For particle reinforced composites, the primitive cubic particle arrangements can be modeled exactly by a conventional cell model with appropriate symmetry and boundary conditions [Fig. 2.20(c)], however, the hexagonal arrangement has to be simulated by approximate cell models [Fig. 2.20(d)]

[17]. The primitive cubic and axisymmetric unit cells have been used in this paper to model two representatives of regular particle arrangements. Further simplifications for 3D modeling are spherical unit cells shown in Figs 2.20(c) and (d) which will be employed, however, for embedded cell modeling.

Embedded cell models

In the present work, 2D and 3D self-consistent embedded cell models will be applied to model the mechanical behavior of composites with random continuous fiber and particle arrangements. Figure 3(a) describes schematically a typical plane strain (2D) embedded cell model with a volume fraction of $f = (d/D)^2$ or axisymmetric (3D) embedded cell model with a volume fraction of $f = (d/D)^3$, where instead of using fixed or symmetry boundary conditions around the fiber-matrix or particle-matrix cell, the inclusion-matrix cell is rather embedded in an equivalent composite material with the mechanical behavior to be determined iteratively in a self-consistent manner.

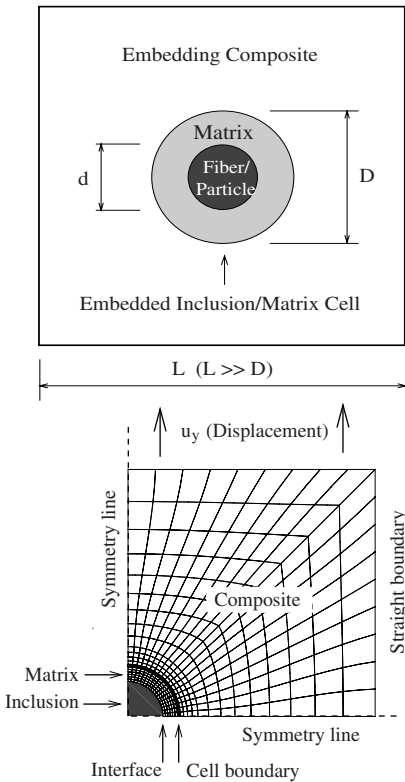


Fig 2.6 (a) Embedded cell model and (b) finite element mesh for an embedded cell model.

If the dimension of the embedding composite is sufficiently large compared with that of the embedded cell, e.g. $L/D = 5$ as used in this paper, the external

geometry boundary conditions introduced around the embedding composite are almost without influence on the composite behavior of the inner embedded cell. Indeed, there exists no difference in the calculated results whether the vertical surfaces are kept unconstrained or remain straight during uniaxial loading.

To investigate the influence of the geometrical shape of the matrix phase on the overall behavior of the composite, different shapes of cross section of the embedded cell were chosen with a circular shaped continuous fiber surrounded by a circular, square, elliptical or rectangular shaped metal matrix (Fig. 2.9). A typical FE mesh and corresponding symmetry and boundary conditions are given in Fig. 2.6(b), where a circular fiber or a spherical particle is surrounded by a circular (for 2D) or spherical (for 3D) shaped metal matrix, which is again embedded in the composite material with the mechanical behavior to be determined.

Iterative modelling procedure

Under axial displacement loading at the external boundary of the embedding composite (Fig. 2.6) the overall response of the inner embedded cell can be obtained by averaging the stresses and strains in the embedded cell or alternatively the reaction forces and displacements at the boundary between the embedded cell and the surrounding volume.

The embedding method is a self-consistent procedure, which requires several iterations as shown in Fig. 2.22.

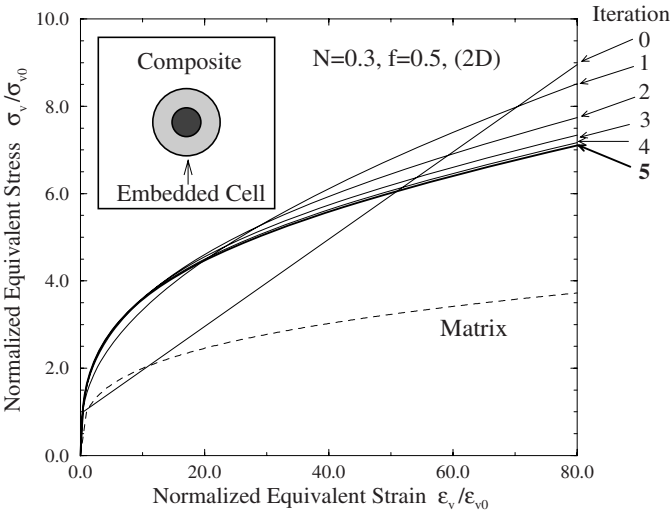


Fig 2.7 Iterative modeling procedure: stress-strain curves for different iteration steps.

An initially assumed stress-strain curve (iteration 0 in Fig. 2.22) is first assigned to the embedding composite, in order to perform the first iteration step. An improved stress-strain curve of the composite (iteration 1) will be obtained by

analyzing the average mechanical response of the embedded cell. This procedure is repeated until the calculated stress-strain curve from the embedded cell is almost identical to that from the previous iteration. The convergence of the iteration occurs typically at the fifth iteration step, as illustrated in Fig. 2.22

It has been found from systematic studies that convergence of the iteration to the final stress-strain curve of the composite is independent of the initial mechanical behavior of the embedding composite (iteration 0). From an arbitrary initial stress-strain curve of the embedding composite the required composite response can be reached after 4-5 iterations for all cases.

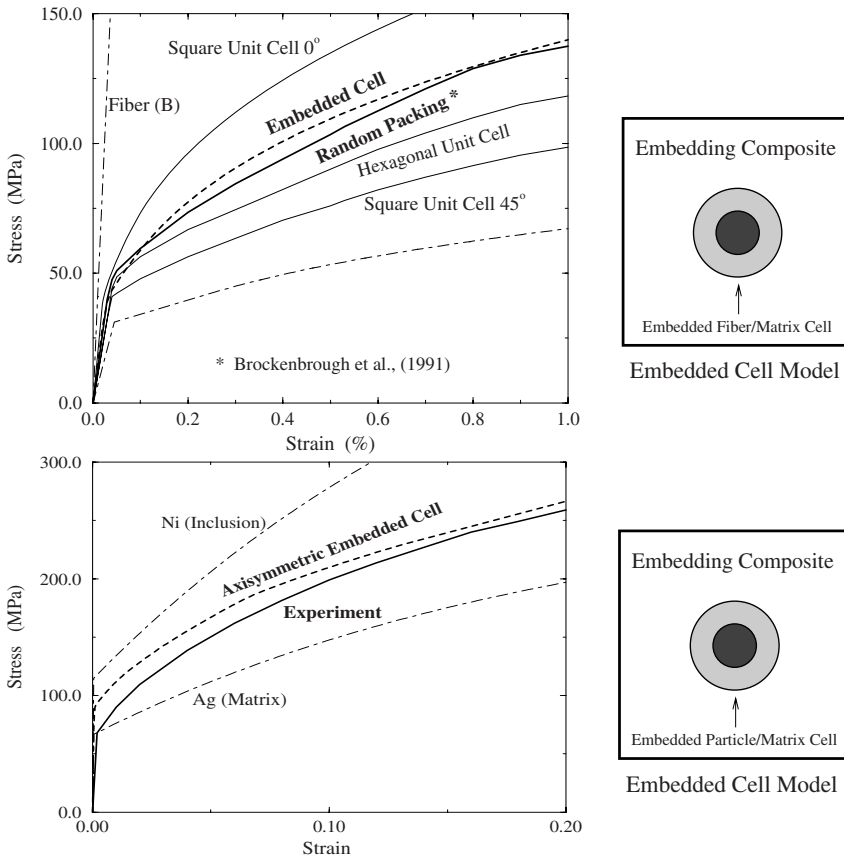


Fig. 2.8 Comparison of the mechanical behavior (a) of an Al-46vol.%B fiber reinforced composite ($N = 1/3$, $f = 0.46$) under transverse loading from different models; and (b) of a Ag-58 vol.%Ni particulate composite from embedded cell model and experiment.

The LARSTRAN finite element program [33] was employed using 8-noded plane strain elements (for 2D) as well as axisymmetric biquadrilateral elements (for 3D) generated with the help of the pre- and postprocessing program PATRAN [34]. A DEC-Alpha work station 3000/300L was used to carry out the calculations,

which typically took 30-50 min to obtain a stress-strain curve with 100-150 loading steps in one iteration loop.

Comparison with experiments

An example of the composite Al 46vol.%B with random fiber packing taken from Ref. [5] has been selected to verify the embedded cell model. This MMC is a 6061-O aluminum alloy reinforced with unidirectional cylindrical boron fibers of 46% volume fraction. The room temperature elastic properties of the fibers are Young's modulus, $E^{(B)} = 410$ GPa, and Poisson's ratio, $\nu^{(B)} = 0.2$. The experimentally determined mechanical properties of the 6061-O aluminum matrix are: Young's modulus, $E^{(Al)} = 69$ GPa, Poisson's ratio, $\nu^{(Al)} = 0.33$, 0.2% offset tensile yield strength, $\sigma_0 = 43$ MPa, and strain-hardening exponent, $N = 1/n = 1/3$.

Figure 5(a) shows a comparison of the stress-strain curves of the composite Al-46 vol.% B under transverse loading from simulations of a real microstructure together with results from different cell models. The stress-strain curve from the embedded cell model employed in this paper shows good agreement with that from the calculated random fiber packing in the elastic and plastic regime, which lies between the curves from square unit cell modeling under 0° loading and hexagonal unit cell modeling.

Furthermore, the stress-strain curve from another experiment [27] on the composite Ag-58vol.% Ni with random particle arrangement (Young's modulus, $E^{(Ni)} = 199.5$ GPa, $E^{(Ag)} = 82.7$ GPa, Poisson's ratio, $\nu^{(Ni)} = 0.312$, $\nu^{(Ag)} = 0.367$, and yield strength, $\sigma^{(Ni)} = 193$ MPa, $\sigma^{(Ag)} = 64$ MPa) has been compared in Fig. 2.8(b) with that from the self-consistent embedded cell model. Good agreement in the regime of plastic response is obtained, although the Ni-particles in the experiment were not perfectly spherical.

These results indicate that the embedded cell model can be used to successfully simulate composites with random inclusion arrangements and to predict the elastic-plastic composite behavior.

Geometrical shape of embedded cell

As mentioned above, different shapes of cross section of the embedded cell model with a circular shaped fiber, as shown in Fig. 2.9(a), are also taken into account to investigate the influence of the geometrical shape of the embedded cells on the overall behavior of the composite. The stress-strain curves of all embedded cell models with different geometrical shapes are plotted in Fig. 2.9(b). With an exception of the square 45° embedded cell model the stress-strain curves are very close for all embedded cell shapes, namely, square- 0° , circular, rectangular- 0° , rectangular- 90° , elliptic- 0° and elliptic- 90° .

From the calculated results of the embedded cell models localized flows have been found around the hard fiber with preferred yielding at 45° . Because of the special geometry of the square 45° embedded cell model with the cell boundary

parallel to the preferred yielding at 45° , the overall stresses of the composite with such a geometrical cell shape are therefore reduced, such that a relative lower stress-strain curve has been obtained from the modeling.

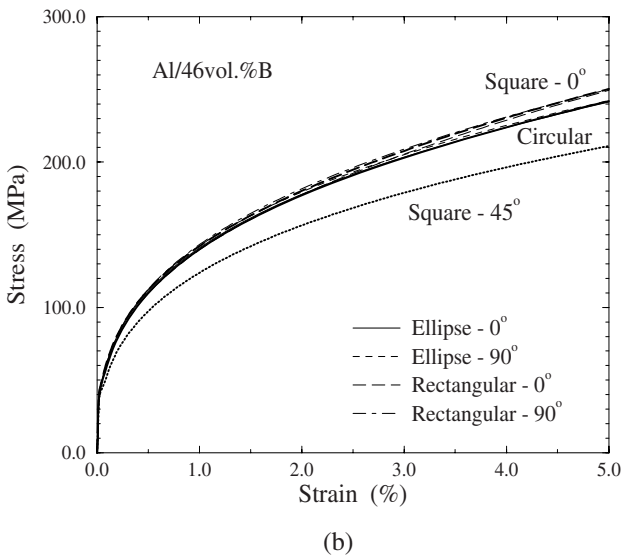
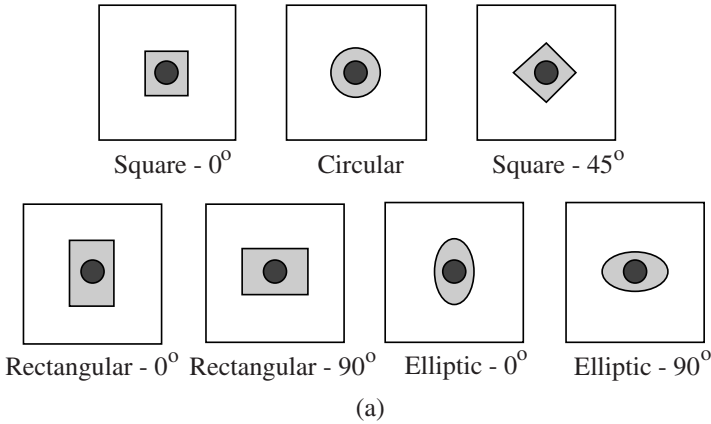


Fig 2.9 Embedded cell models: influence of (a) different matrix shapes on (b) stress-strain curves for an Al-46vol.%B ($N = 1/3$, $f = 0.46$) composite.

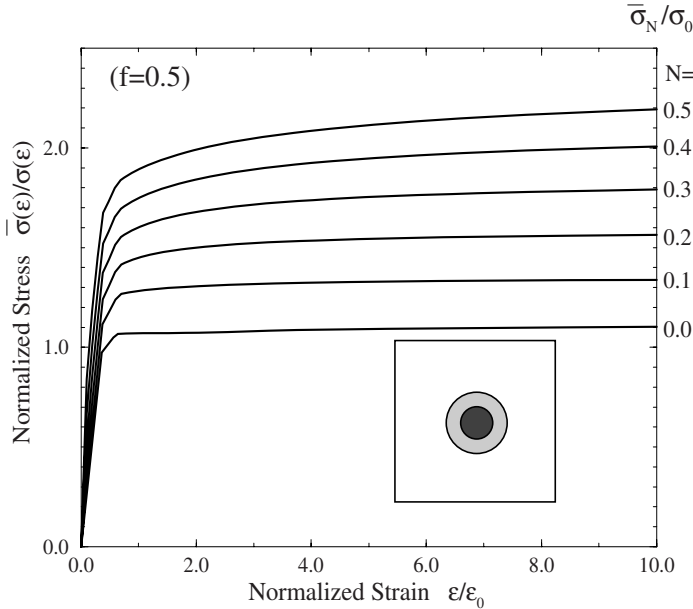
The almost identical responses of all other embedded cell models indicate that, besides the special shape of matrix with 45° cell boundaries, the predicted mechanical behavior of fiber reinforced composites under transverse loading is independent of the modeling shape of the embedded composite cell. That allows us to employ any embedded cell shape to model the mechanical behavior of the

composite with random fiber arrangement. In the following systematic studies the circular shaped embedded cell model with circular cross section of rigid fiber will thus be taken to predict the general transverse mechanical behavior of the composite with random fiber arrangement. In the same way, a spherical shaped embedded cell model containing a spherical particle will be used to predict the axial mechanical behavior of composites with random particle arrangement.

2.1.2 Systematic studies with self-consistent embedded cell models

Composite strengthening is dependent on fiber and particle arrangement, inclusion volume fraction and the matrix strain-hardening exponent. The effect of fiber and particle arrangement is best demonstrated by considering different cell models. The effect of the inclusion volume fraction has been taken into account by applying different ratios of the circular (2D) and spherical (3D) matrix and the inclusion in the embedded cell model.

The effect of the matrix strain hardening exponent has been investigated by changing the parameter, N , of the material hardening law for the matrix in equation (2.1). Some results from the systematic studies with embedded cell models are given in Figs 2.10-2.13.



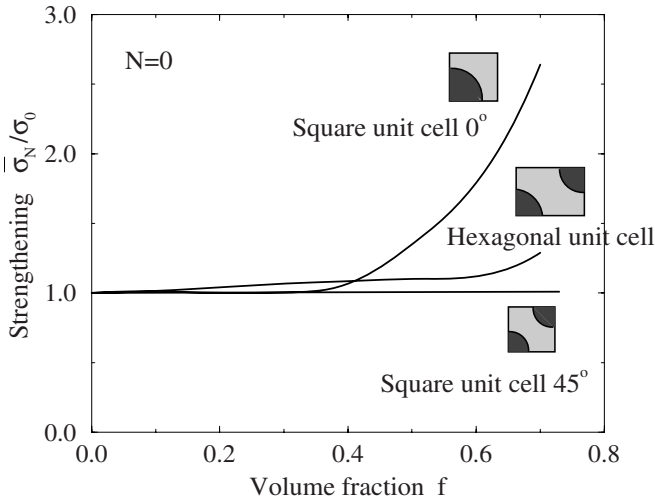


Fig 2.10 (a) Normalized stress-strain curves from embedded cell models (2D) for different N -values ($f=0.5$) and (b) composite strengthening from different cell models (2D, $N=0$).

The influence of matrix strain-hardening is shown in Figs 2.10(a) and 2.11(a). The predicted transverse (2D) and axial (3D) overall stress-strain curves (normalized by yield stress and yield strain of the matrix, respectively) for the case of strain-hardening exponents between $N = 0.0$ and 0.5 are depicted in Fig. 2.10(a) (2D) for a fiber volume fraction $f = 0.5$ and in Fig. 2.11(a) (3D) for a particle volume fraction of $f = 0.4$. At sufficiently large strains (e.g. at $E = 10$), the normalized overall stresses approach constant values, i.e. composite strengthening levels, as illustrated on the right-hand side of Figs 2.10(b) and 2.11(b) for $\bar{\varepsilon} = 10\varepsilon_0$. The strength of the composite is seen to increase with N and similar trends of nearly linear increase with N are found for all particle volume fractions, f [Figs 2.11(a) and 2.13].

The dependence of composite strengthening on inclusion volume fraction obtained by the self-consistent embedded cell modelling is shown in Fig. 2.10(b) for a non-hardening matrix with continuous fiber reinforcement and in Fig. 2.11(b) for a strain-hardening matrix ($N = 0.2$) with particle reinforcement. For comparison, the corresponding values of composite strengthening for regular fiber and particle arrangements taken from unit cell modelling and from two approximate models, namely Duva's model [28] and the modified Oldroyd model [26,27] are also drawn as a function of fiber and particle volume fraction in these figures, respectively. A detailed discussion of this comparison is given in Ref. [27].

Duva's model is a self-consistent model and valid particularly in the dilute regime, $f < 0.2$. Composite strengthening by the Duva model is given as Composite strengthening levels of the modified Oldroyd model are taken from Ref. [27].

$$\frac{\bar{\sigma}_N}{\sigma_0} = (1 - f)^{-(2.11N + 0.39)} \quad (2.8)$$

A summary of the dependence of composite strengthening on inclusion volume fraction and matrix strain-hardening for randomly arranged continuous fibers and particles is depicted in Figs 2.12 and 2.13(a) for matrix strain-hardening exponents $N = 0.0$ - 0.5 , and compared with predictions from 2D and 3D unit cell models. In addition, a comparison with predictions from Duva's model and the modified Oldroyd model for the case of particle reinforced composites is shown in Fig. 2.13(b).

For continuous fiber reinforced composites with a non-hardening matrix the hexagonal arrangement provides slightly higher transverse composite strengthening over the square arrangement at volume fractions $f < 0.5$, whereas the random arrangement from the embedded cell model supplies an intermediate value between the two regular arrangements except at volume fraction $0.38 < f < 0.5$ (Fig. 2.12). At volume fractions $0.38 < f < 0.5$, the random arrangement from the embedded cell model possesses the lowest composite strengthening level. On the contrary, the composite strengthening of the square arrangement is higher than that of the hexagonal arrangement for volume fractions $f > 0.4$. For the composite with a small exponent of strain-hardening matrix, $N < 0.2$, similar relations among the three arrangements were found, with the cross points of any two curves being closer to $f = 0$ with increasing N . For composites with a higher strain-hardening exponent of the matrix, $N > 0.2$, the strengthening values are almost the same for the three arrangements considered at volume fractions $f < 0.2$. At volume fractions $f > 0.2$, the square arrangement provides again the highest strengthening and the hexagonal arrangement the lowest strengthening. A comparison of composite strengthening in Fig. 2.12 for three continuous uniaxial fiber arrangements can be summarized as follows: in the case of low strain-hardening of the matrix, composites with hexagonal fiber arrangement behave stronger than those with random fiber arrangement, which behave, however, at low volume fractions stronger than those with random arrangement. With increasing strain-hardening ability of the matrix, the composites of all three arrangements behave similarly at low fiber volume fractions. At higher inclusion volume fractions the difference in composite strengthening is becoming larger, with the square arrangement possessing the highest, the random arrangement the intermediate and the hexagonal arrangement the lowest level.

The stress and strain distributions in a typical embedded cell model (2D) are shown in Fig. 2.14. In the embedded cell the localized flow stresses with preferred yielding in the 45° direction are seen apparently around the hard fiber and extending into the embedding composite in the vicinity of the embedded cell.

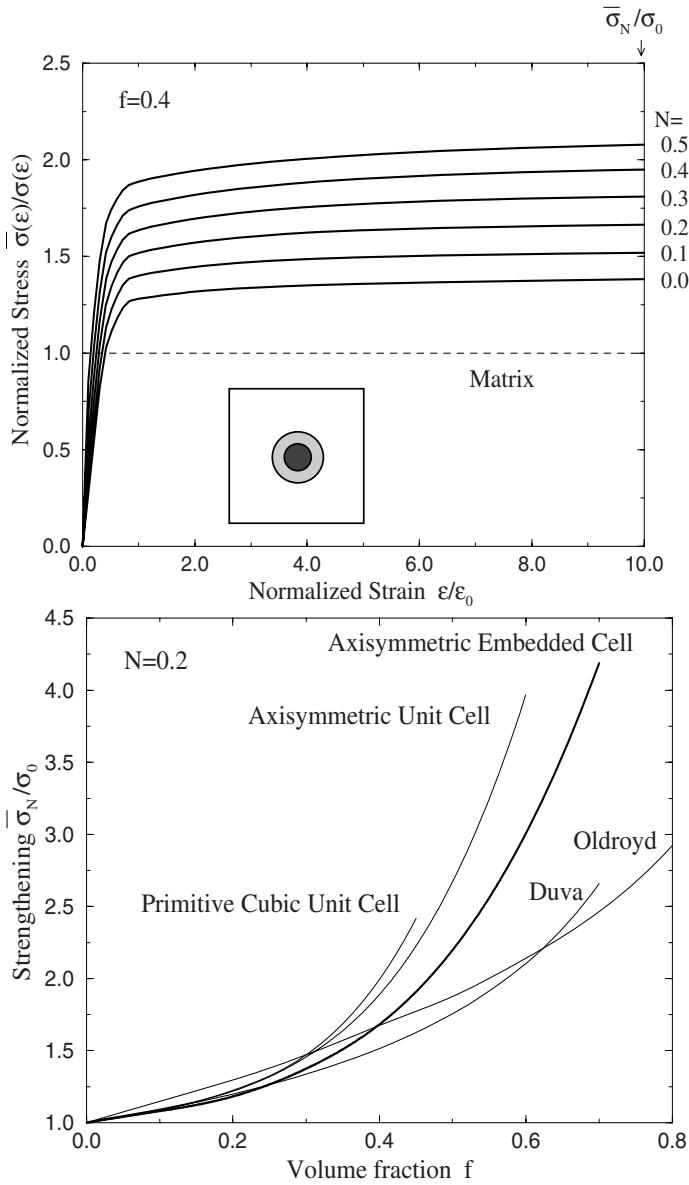


Fig. 2.11 (a) Normalized overall composite stress-strain curves from axisymmetric embedded cell models (3D) for different N -values ($f = 0.4$) and (b) composite strengthening for matrix strain-hardening $N = 0.2$ from different cell models (3D).

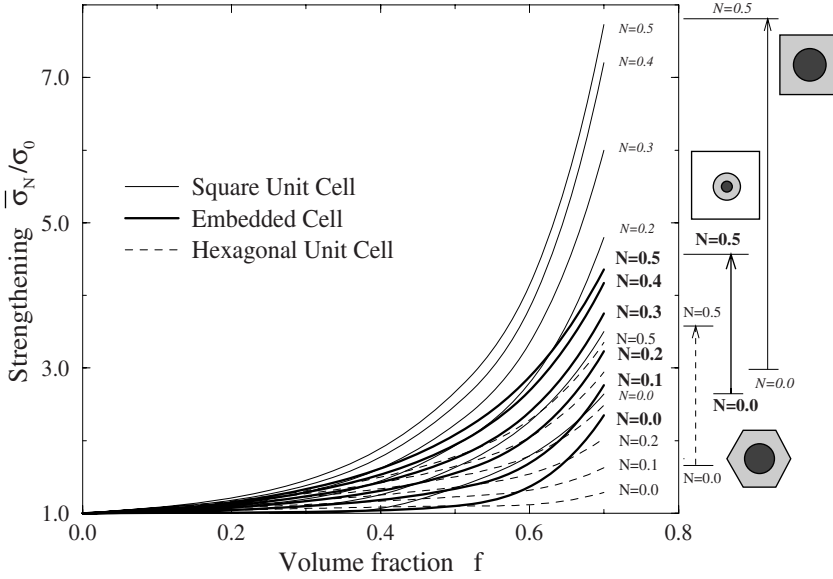


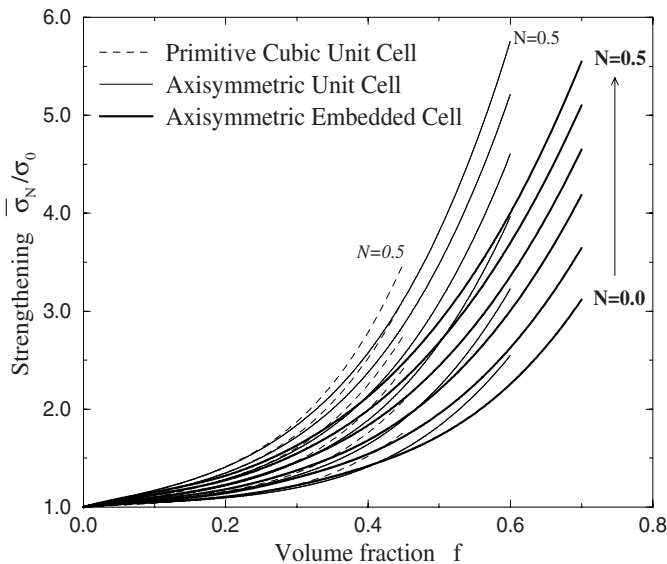
Fig 2.12 Comparison of composite strengthening by continuously aligned fibers from different 2D cell models: embedded cell model, square and hexagonal unit cell model.

It characterizes the local response of the composite under transverse loading. However, the stresses and strains are homogeneously distributed in the embedding composite far from the embedded cell. This represents the overall behavior of the corresponding composite. In the case of random fiber arrangement, the situation around every single fiber is, of course, more complicated. However, the real situation can be considered in average as a fiber-matrix cell surrounded by corresponding equivalent composite material, which represents the average overall composite behavior.

From comparisons for particle reinforced composites in Figs 2.28(a) and (b) it can be seen that the composite strengthening levels from the primitive cubic, the axisymmetric unit cell models and the self-consistent axisymmetric embedded cell models are very close at low particle volume fractions, f , and low matrix strain-hardening exponents, N . With increasing particle volume fraction, f and matrix strain-hardening exponent, N , the strengthening level of the composites increases for all the models considered. However, the primitive cubic unit cell provides the highest composite strength, while the self-consistent axisymmetric embedded cell predicts the softest composite response among these three models. This effect can be explained by considering the constraint of neighbouring particles through the necessary strict boundary conditions of the models with regularly arranged particles. As the particle volume fraction increases, the distance between the particles decreases until they touch at a volume fraction of $f = 0.5236$ for the primitive cubic cell model (primitive cubic particle arrangement), and a volume fraction of $f =$

2/3 for the axisymmetric cell model (hexagonal particle arrangement). In the self-consistent axisymmetric embedded cell model the particles remain surrounded by the matrix up to an extreme volume fraction of $f = 1$, as seen in Fig. 2.6. The equivalent composite surrounding the embedded inclusion-matrix cell provides thus less constraint on the inclusion-matrix cell compared to conventional unit cell models of the same volume fraction. In most practical relevant composites, the inclusions are randomly arranged and on average, no such restricting constraints exist as in the regular primitive cubic and hexagonal arrangements. For this reason, the self-consistent axisymmetric embedded cell model is believed to be the most realistic approximation to the geometry of real composites containing randomly arranged spherical particles.

At low particle volume fractions ($f < 0.2$) and low matrix strain-hardening ability ($N < 0.2$) the composite strengthening levels from the present selfconsistent axisymmetric embedded cell model and the Duva model are very similar. With increasing particle volume fraction, f , the differences in composite strengthening between these two models are significant for low matrix strain-hardening ability, however, for $N \sim 0.5$ the two strength predictions are comparable. The modified Oldroyd model provides a very narrow distribution of composite strengthening with respect to N of matrix strain-hardening and an almost linear strength dependence on particle volume fraction, f . Good agreement between the self-consistent axisymmetric embedded cell model and the modified Oldroyd model exists only at low volume fractions and high strain-hardening rates ($N \sim 0.5$) of the matrix.



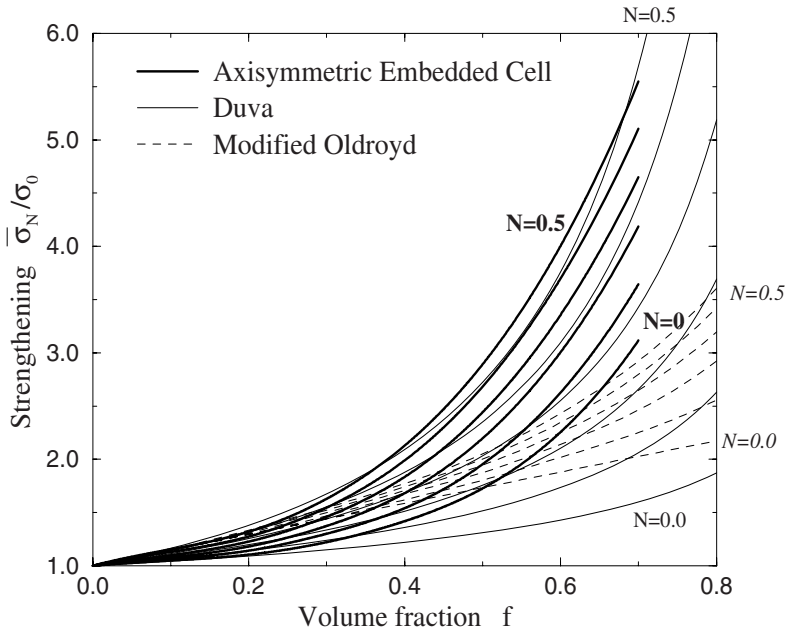


Fig 2.13 Comparison of composite strengthening by spherical particles from different 3D cell models: (a) embedded cell model, primitive cubic and axisymmetric unit cell model and (b) embedded cell model, Duva model and Oldroyd model.

From above comparisons between the models it is clear that at low particle volume fractions ($f < 20\%$) the strengthening of metal matrix composites reinforced with randomly or regularly arranged particles can be predicted with either the axisymmetric unit cell model, the embedded cell model or the simple Duva model. However, for higher particle volume fractions the self-consistent embedded cell model should be applied to obtain the overall mechanical response of technically relevant composites reinforced by randomly arranged spherical particles

Strengthening Model

The strength of MMCs reinforced by hard inclusions under external mechanical loading has been shown to increase with inclusion volume fraction and strain-hardening ability of the matrix for all inclusion arrangements investigated. From the presented numerical predictions a strengthening model for aligned continuous fiber reinforced MMCs with random, square (0°) and hexagonal arrangements, as well as for spherical particle reinforced MMCs with random, primitive cubic and hexagonal arrangements, can be derived as a function of the inclusion volume fraction f , and the strain-hardening exponent, N , of the matrix [31]:

$$\bar{\sigma}_N = \sigma_0 \left[\left(1 - \frac{f}{c_1(2-N)} \right)^{-(c_2 N + c_3)} - c_4 \left(f + \frac{N}{5} \right) \right] \quad (2.9)$$

where σ_0 is the matrix yield stress, and c_1, c_2, c_3 and c_4 are constants summarized in Table 2.1



(a)



(b)

Fig 2.14 (a) Equivalent stress and (b) effective plastic strain in an embedded cell model with circular rigid fiber ($f = 0.5$) and metal matrix ($E = 100$ GPa, $\epsilon_0 = 0.1$ %, $\sigma_0 = 100$ MPa, $N = 0.2$) at 3.8% total strain.

Equation (2.10) represents best fits to the calculated composite strengthening values C_y for matrix strain-hardening exponents N in the limit of $0.0 < N < 0.5$ for square 0° , hexagonal and random fiber arrangements, respectively, and fiber volume fractions, f in the range of $0.0 < f < 0.7$. A comparison of this strengthening model [equation (2.10)] for random fiber arrangements with the values calculated by using self-consistent embedded cell models shows close agreement with an average error of 1.25% and a maximum error of 6.95% [31].

Table 2.1:
Constants for strengthening models

	c_1	c_2	c_3	c_4
2D				
Self-consistent embedded cell model	0.361	1.59	0.29	0.1
(Random fiber arrangement)	0.405	2.35	0.65	0.22
Square unit cell model (0°)	0.305	1.3	0.05	0.0
Hexagonal unit cell model				
3D				
Self-consistent axisymmetric embedded cell model	0.45	2.19	0.84	0.53
(Random particle arrangement)	0.34	2.3	0.65	0.5
Primitive cubic unit cell model	0.38	2.5	0.7	0.66
Axisymmetric unit cell model				

Equation (2.10) is also available for matrix strain-hardening exponents N in the limits of $0.0 < N < 0.5$ for self-consistent axisymmetric embedded cell models (particle volume fractions f in the range of $0.05 < f < 0.65$ with an average error of 1.59% and a maximum error of 6.68% for the extreme case $f = 0.05$, $N = 0.5$), axisymmetric unit cell models (particle volume fractions f in the range of $0.05 < f < 0.55$ with an average error of 1.22% and a maximum error of 6.18% for the extreme case $f = 0.55$, $N = 0.5$) and for primitive cubic unit cell models (particle volume fractions f in the range of $0.05 < f < 0.45$ with an average error of 1.43% and a maximum error of 6.38% for the extreme case $f = 0.05$, $N = 0.5$).

Conclusions

The transverse elastic-plastic response of metal matrix composites reinforced with unidirectional continuous fibers and the overall elastic-plastic response of metal matrix composites reinforced with spherical particles have been shown to depend on the arrangement of reinforcing inclusions as well as on inclusion volume fraction f , and matrix strain-hardening exponent, N . Self-consistent plane strain and axisymmetric embedded cell models have been employed to predict the overall mechanical behavior of metal matrix composites reinforced with randomly arranged

continuous fibers and spherical particles perfectly bonded in a power law matrix. The embedded cell method is a self-consistent scheme, which typically requires 4-5 iterations to obtain consistency of the mechanical behavior in the embedded cell and the surrounding equivalent composite. Experimental findings on an aluminum matrix reinforced with aligned but randomly arranged boron fibers (Al-46 vol.% B) as well as a silver matrix reinforced with randomly arranged nickel inclusions (Al-58 vol.% Ni) and the overall response of the same composites predicted by embedded cell models are found to be in close agreement. The strength of composites with aligned but randomly arranged fibers cannot be properly described by conventional fiber-matrix unit cell models, which simulate the strength of composites with regular fiber arrangements.

Systematic studies were carried out for predicting composite limit flow stresses for a wide range of parameters, f and N . The results for random 3D particle arrangements were then compared with regular 3D particle arrangements by using axisymmetric unit cell models as well as primitive cubic unit cell models. The numerical results were also compared with those from the Duva model and from the modified Oldroyd model. The strength of composites at low particle volume fractions has been shown to be in very close agreement except for the modified Oldroyd model. With increasing particle volume fractions, f , and strain hardening of the matrix, N , the strength of composites with randomly arranged particles cannot be properly described by conventional particle-matrix unit cell models, as those are only able to predict the strength of composites with regular particle arrangements.

Finally, a strengthening model for randomly or regularly arranged continuous fiber reinforced composites under transverse loading and particle reinforced composites under axial loading is derived, providing a simple guidance for designing the mechanical properties of technically relevant metal matrix composites: for any required strength level, equation (2.10) will provide the possible combinations of particle volume fraction, f , and matrix hardening ability, N . Thus, for the near future, strong impact of the present work on the development of new particle reinforced metal matrix composites is expected.

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2.2 Multiphase finite elements

2.2.1 3D multiphase finite element method²

Introduction

Inhomogeneous stress distributions which occur as a result of the interaction of the individual microstructural constituents in multiphase materials are frequently simulated with the finite-element (FE-) method [1]. Such microstructural analyses contribute to the understanding of the stress and strain distributions in each constituent and can be used to depict critical loads or critical configurations. So far, FE modelling of realistic microstructures is essentially limited to 2D-models [2-5]. However, 2D-simulations are not able to represent the morphological complexity of a realistic 3D-microstructure. Inhomogeneities located underneath the surface of a modelled microstructure as well as the inherent 3D-nature of the microstructure may introduce significant changes in comparison to 2D-simulations. Therefore, fully 3D-analyses are currently requested in order to evaluate the predictions based on 2D-simulations. FE-modelling of two-phase materials based on single-phase elements is limited to the simplest 3Dstructures such as single inclusions or regular microstructures [6-10]. Conventional 3D-modelling of realistic microstructures is practically impossible since it would require fantastically complex FE meshes.

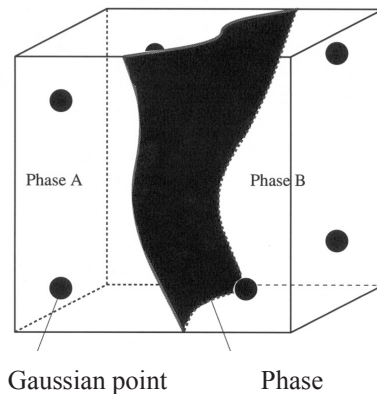


Fig. 2.15 8-node hexahedral multiphase element with bilinear interpolation and full integration.

The first 3D-simulations of more realistic microstructures have been reported by Hollister and Kikuchi [11]. They applied digital image based modelling for the

² Reprinted from N. Lippmann, Th. Steinkopff, S. Schmauder, P. Gumbsch, "3D-Finite-Element-Modelling of Microstructures with the Method of Multiphase Elements", Computational Materials Science 9, pp. 28-35 (1997), with kind permission from Elsevier

micromechanical study of bone tissues. A 3D-model is developed by combining 2D-images. Each pixel in a 2D-image is recognized as a voxel which is identified as a finite element in the analysis.

Recently, the method of multiphase elements (MME) where the Gaussian points of one finite element can be assigned to different material properties has been successfully applied for the 2D-simulation of realistic microstructures [2-5]. Multiphase elements were introduced since the reconstruction of phase boundaries with irregular shape in singlephase FE-models is very complicated. The main advantage of the multiphase elements over conventional singlephase elements are the flexibility in the construction of the FE-model as well as the numerical efficiency. Based on our experiences with this method, the new 3D-multiphase element has been developed in the framework of the non-linear FE-code LARSTRAN [12]. The 3D-multiphase element is defined for the following element types:

- 8-node hexahedral elements with trilinear interpolation and full integration (eight Gaussian points, Fig. 2.15).
- 27-node and 20-node hexahedral elements with triquadratic interpolation (Gaussian points).

Method

Consider the main ideas of the MPFE (multiphase finite element) method. Commonly, each element of the FE mesh is attributed to one phase; the same material properties are assigned to all integration points of an element and the phase boundaries are supposed to coincide with the edges of finite elements. The idea of the method of multiphase elements is that the different phase properties are assigned to individual integration points in the element. Therefore, the FE mesh in this case is independent of the phase arrangement of the 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 simulation of the mechanical behaviour of materials with complex microstructure is the main advantage of the method of multi phase elements.

In the case of 3D simulations of the mechanical behaviour of heterogeneous materials with arbitrarily arranged phase boundaries, it is almost impossible to construct the FE mesh in such a way that the edges of finite elements correspond to the phase boundaries. Therefore, the possibilities, which the multiphase element method offers are especially important in the 3D case.

In the 3D MPFE code, finite elements of low order (with linear or square interpolation functions) are used. The form and distribution of the phases are introduced automatically in the FE model from digitised micrographs of the microstructure.

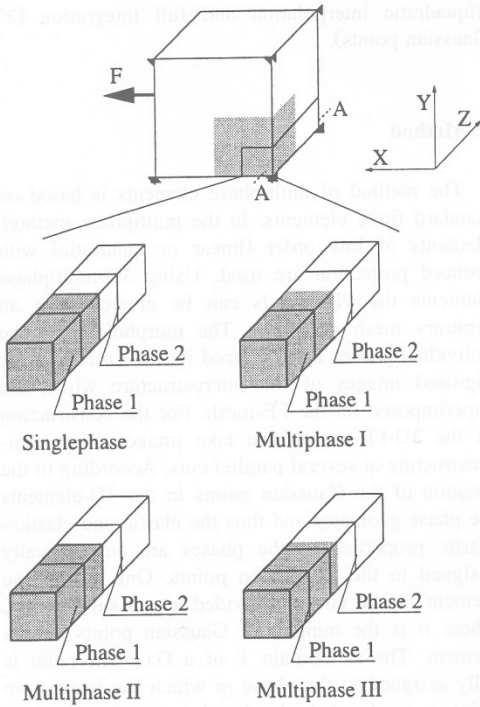


Fig 2.16 FE-models for the verification of the multiphase elements.

Several material layers are metallographically removed equidistantly from the surface of the specimen by careful polishing. Micrographs from each polished surface are made. The thickness of the removed layers must be known for each layer as exactly as possible. Then, the micrographs are digitised with the use of image analysis software, and the 3D real structure of the material is reconstructed from the digitised micrographs of the sections.

Each pixel in 2D digitised micrograph is assigned to some volume of material, and therefore determines the correspondence of Gaussian points to the phases in the material. The mechanical properties of the phases are automatically assigned to the integration points.

One multiphase element can be virtually divided into n subdomains, where n is the number of Gaussian points in this element. The subdomain k of a Gaussian point is fully assigned to the phase in which the integration point r_k is located. A closed integration (e.g. to provide the stiffness) in the multiphase element is not possible. Therefore, the Gaussian quadrature, which is the weighted summation of the function values at selected integration point's x_k , is used as integration scheme:

$$\int f(x)dx = \sum_k w_k \cdot f_{vk}(x_k) \quad (2.10)$$

The weights w_k correspond to the volume of the subdomains and f_{vk} indicates that the function for the phase v of the subdomain k is used.

In the following, the reliability of the 3D-multiphase elements is studied by 3D-FE-modelling of a simple model and subsequent comparison with the results of singlephase FE-modelling. In this case we investigate the influence of a strong stress jump on the simulations. Furthermore, the development of a 3D-model of a realistic two-phase microstructure is presented. Finally, the results of this simulation are compared with the results of a 2D-simulation of a representative intersection of the microstructure.

Examples

Stress distribution due to a cubic inclusion in a matrix

The method of multiphase elements would usually be not applied to the modelling of such simple geometries as the cubic inclusion in a matrix which is presented in this first example. However, since this geometry can also be modelled by single-phase FE's it is suitable to demonstrate both the reliability as well as limitations of the multiphase elements by a direct comparison of both methods. A small number of elements in the models permit an intensive evaluation of results.

A cubic inclusion (phase 1) with an edge length 1 is embedded into an Al-matrix (phase 2) cell of the size 21 x 21 x 21 (Fig. 2.16). In this linear-elastic calculation the Young's modulus of Silicon (168.2 GPa) [13] is assumed for the inclusion and 70 GPa for the matrix (Al). The Poisson ratios of the matrix and inclusion are chosen to be 0.3 and 0.25, respectively. Boundary conditions are imposed which simulate the stress distribution in the model under uniaxial tension and plane strain conditions (symmetric boundary conditions). The 3D-models (see Fig. 2.16) are created with 20-node hexahedral elements as follows:

(1) A singlephase model with connected nodes at the phase boundary which has 64 conventional elements.

(2) The multiphase I model consisting of 27 multiphase elements. The central nodes of the multiphase elements containing the phase boundary are located on the phase boundary.

(3) The multiphase II model corresponds to the singlephase model in the number of elements and discretisation. The phase boundary is located at the element edge.

(4) Model multiphase III comprises 36 multiphase elements of various sizes. The phase boundary is located between the nodes and Gaussian points of the elements containing the phase boundary.

The row of elements along the z -axis in Fig. 2.16 is chosen to evaluate the maximum stress-component σ_x , for which a pronounced stress jump is expected at

the phase boundary. The edge length of the elements is equivalent in x - and y -direction in all models to eliminate additional effects of stress gradients. Both, the results at the Gaussian points as well as the element averaged results are evaluated.

Results at the Gaussian points

Fig. 2.17 shows the calculated maximum normal stress σ_x along the z -direction (cf. Fig. 2.16, path A-A) for the Gaussian points with the lowest x - and y -distance to the z -axis. Generally, the same behaviour in the inclusion and matrix is observed in all simulations.

The stresses in the inclusion (phase 1) increase with decreasing distance to the phase boundary. The largest difference (less than 10%) occurs between single-phase and multiphase III model. The stress jump at the phase boundary is almost identical in the singlephase and the multiphase II simulation. Depending on the nearest distance of a Gaussian point to the phase boundary a more or less steep stress gradient is obtained in multiphase III and multiphase I simulations. The stresses in the matrix increase with the distance from the phase boundary.

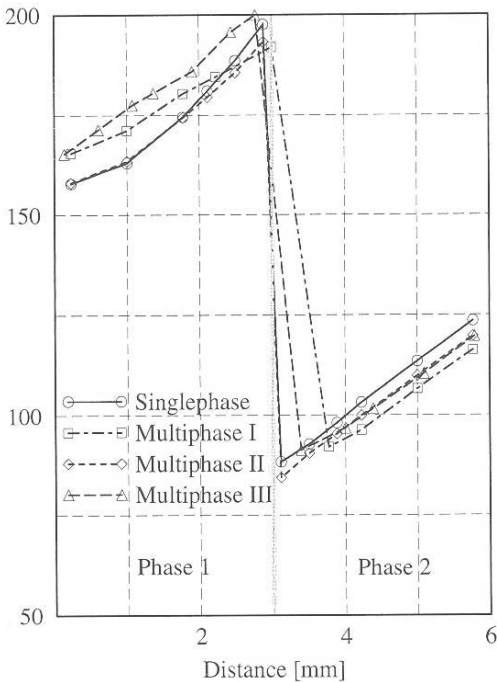


Fig 2.17 Results at the Gaussian points.

Element averaged results

Element averaged results (Fig. 2.18) which are used in post-processors such as PATRAN³ to produce fringe plots are calculated on the basis of the averaged results at the nodes.

Almost equivalent values of stresses are obtained for the singlephase and multiphase II simulations whereas in the multiphase I and III simulations the stress jump is not sufficiently reproduced. Since different material properties occur in these multiphase elements the stress maxima or minima are ‘smeared’ in the phase boundary region. This behaviour can not be avoided but reduced by using smaller elements where either the matrix or the inclusion dominates in the calculation of the averaged results.

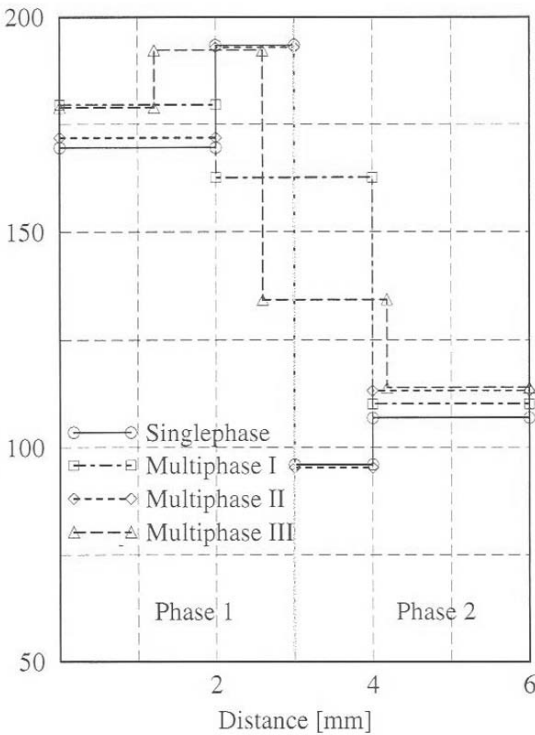


Fig 2.18 Element averaged results.

Comparison of a 2D- and 3D-simulation of a realistic microstructure

As an example of a more realistic application of multiphase elements, the microstructural behaviour of an AlSi-cast alloy is simulated in a 3D-FE-model and

³ PDA Engineering, 2975 Redhill Avenue, Costa Mesa, California 92626, USA

compared with a 2D-simulation. In order to describe appropriate macroscopic boundary conditions, embedded cell simulations [4] are performed. A 3D-model of size $240 \times 240 \times 30 \mu\text{m}$ is generated as follows (Fig. 2.19):

- The central region of the model of size $120 \times 120 \times 30 \mu\text{m}$ with 9600 g-node hexahedral elements (c.f. Fig. 2.19(1)) is used for the simulation of the two-phase microstructure.
- The microstructure in the model is developed on the basis of 4 intersections of the microstructure at each $10 \mu\text{m}$ starting from the surface of the specimen.

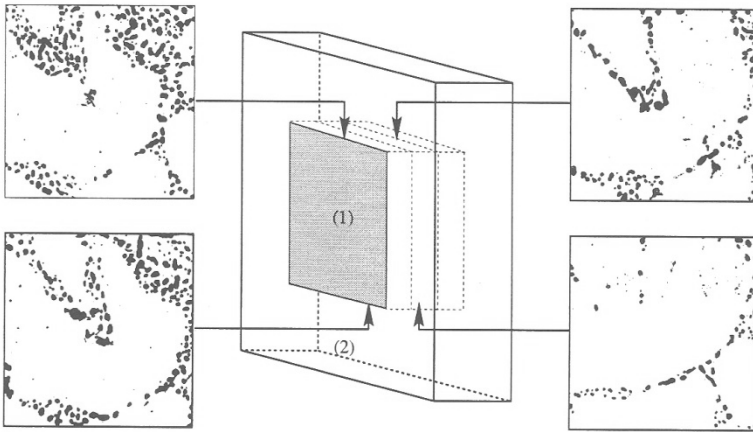


Fig 2.19 Generation of the 3D-multiphase model (schematically)

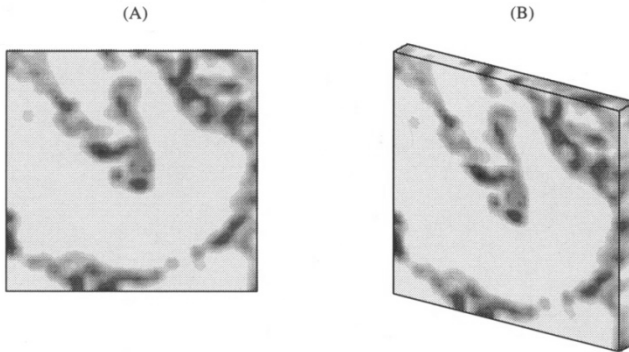


Fig 2.20 Designation of the phases to the elements: (A) 2D-FE model, (B) 3D-FE model

- The cell representing the microstructure is surrounded by 7296 single phase g-node hexahedral elements (c.f. Fig. 2.19(2)).

- All nodes at the free surfaces are fixed in z-direction (perpendicular to the model surface) to obtain appropriate plane strain boundary conditions.

The actual FEZ-mesh used in the calculations is given in Ref. [14]. For comparison to the 3D-simulation, a 2D-multiphase model of size 240 x 240 μm is created:

- With 1600 4-node quadrilateral plane strain elements in the central region. The edge length of these elements is equal to the edge length in the 3D-model.
- The two-phase microstructure in this model is chosen according to one of the intersections which are considered in the 3D-model ($z = 10 \mu\text{m}$). The cell which represents the microstructure is surrounded by 1216 4-node quadrilateral elements.

Table 2.2
Elastic-plastic material properties of the constituents

Property	Al-Matrix	Al/Si7Mg
Yield stress σ_0	218 MPa	250 Mpa
Yield strain ε_0	0.325 %	0.357%
Constitutive relation	$\sigma = \sigma_0(\varepsilon / \varepsilon_0)^{0,14}$	$\sigma = \sigma_0(\varepsilon / \varepsilon_0)^{0,08}$

The linear-elastic material properties in both models are imposed according to Section 3.1. Additionally, the constitutive relation for the simulation of the elastic-plastic properties of the Al-matrix and the AlSi7Mg-alloy (surrounding) are given in table 2.2. The constitutive relation for the AlSi7Mg-cast alloy was determined from experimental stress-strain diagrams. The mechanical properties of the matrix were determined separately from a macroscopic specimen with the chemical composition of the matrix.

The preprocessing for the 3D-model is almost the same as for the simple model with the inclusion, which demonstrates the efficiency of the method of multiphase elements in the preprocessing stage. This efficiency of model construction is needed for the 3D-analyses of realistic microstructures.

The designation of phase properties to the elements is depicted in Fig. 2.20 for both models. The color-coding is proportional to the number of Gaussian points in the phase: the darker the color the more Gaussian points of the element are assigned to silicon. The phase distribution in the 2D- and 3D-model is equivalent, since the same discretisation is used in both models.

The resulting stress distributions (σ_x Fig. 2.21) for both models show stress concentrations in the Si-eutectic as a result of the higher stiffness of Silicon. The maximum stresses σ_x and the extension of the stress maxima are somewhat higher in the 3D-model. However, generally the stress distributions are almost identical for both models. This may be understood as a result of the simulated microstructure, where large matrix cells exceeding the model dimension in z-direction are surrounded by Si-eutectic.

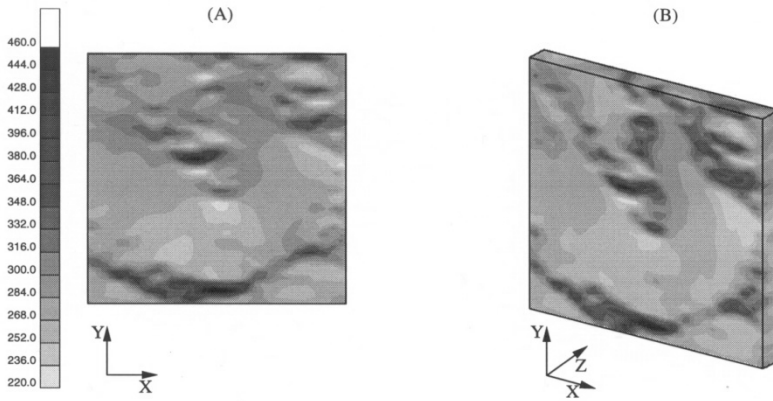


Fig 2.21 Stress distribution σ_x , loading axis corresponds to x-axis: (A) 2D-FE model, (B) 3D-FE model.

Since the model is limited to an intersection of such a cell, the material properties do not change significantly in the third dimension.

The results presented here are the first applications of the 3D-multiphase elements. In the future, we plan a direct comparison of 3Dsimulations with experiments on the basis of displacement fields. The displacements determined experimentally in the scanning electron microscope during the in-situ deformation of an AlSi-specimen are directly compared to the displacements calculated in a 3D-microstructural simulation of these experiments.

Conclusions

A 3D-multiphase element was introduced which enables the 3D-analysis of realistic microscopic as well as macroscopic structures. A simple inclusion model was used to demonstrate the reliability of 3D-multiphase elements by direct comparison with a 3D-singlephase model. The results obtained for the Gaussian points show very good agreement between singlephase and multiphase simulations.

Compared to the digital image based modelling (singlephase method, voxels) [11] the multiphase method distinguishes the different phases with better resolution, since the smallest unit to represent the second phase is the Gaussian point. Thus, even the effect of particles which are smaller than the element size can be taken into account in calculating stress distributions. In the case of equivalent mesh density the volume fraction of phases is more accurately reproduced in the multiphase method. Advantages of the multiphase elements in comparison to the conventional FE-modelling are:

- Higher flexibility of the models because one regular mesh can be used for the simulation of any microstructure.

- Increased resolution of material gradients since different constitutive relations can be used in one element.
- Easier assignment of failure criteria when crack initiation and crack propagation is modelled because those can be based on individual Gaussian points.
- Increased numerical efficiency: if one would decompose one 8-node multiphase hexahedral element with eight Gaussian points into eight 8-node singlephase elements, the CPU-time for the calculation would be about 16-times higher in the singlephase simulation.

The element averaged results obtained in the multiphase simulation differ from the singlephase results: as a consequence of the different material properties in the elements stress concentrations are reduced and stress jumps are 'smeared'. For certain applications this is actually intended; among them are gradient materials. The 3D-multiphase elements seem to be a tool for the stress-strain analysis of complex and irregular 3D-microstructures. However, occurrences at phase boundaries such as debonding can not be simulated with this method.

Finally, the creation of a 3D-model of a realistic microstructure was presented. This model shows the efficiency of the method of multiphase elements with respect to preprocessing and a realistic stress analysis of complex heterogeneous materials. In comparison to the 2D-simulation the maximum normal stresses in the 3D-simulation are somewhat higher for the simulated microstructure. We assume that in the case of microstructures with isolated particles the results of 2D- and 3D-simulations will differ more significantly.

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2.2.2 Multiphase finite element method and damage analysis⁴

In this work, the possibilities of the methods of multiphase finite elements [1-5] and element elimination technique (EET) for studying the damage initiation and evolution, and fracture in two-phase materials for both 2D and 3D cases are discussed.

Element elimination technique and generalised damage parameter

Conditions of the element elimination: Generalised damage parameter

The element elimination technique (EET), described in Chapter 3 in more details, is based on the quasi-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 displacement) 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.

A criterion of element elimination which is appropriate for each material should be chosen by comparison of numerical and experimental results as well as by experimentally studying micromechanisms of damage initiation. For instance, Wulf used the condition of critical plastic strain as criterion for element elimination [3]. Lippmann et al. [9] and Hönle et al. [10] have used a two-criteria model of element elimination for the simulation of Al/Si cast alloys: elements which were assigned to hard (Si) particles were eliminated on the basis of a normal stress criterion, and the critical value for failure of the ductile matrix phase was simulated using a damage-parameter, which is based on the work of Rice and Tracey [11] and Hancock and Mackenzie ([12], see also [13]). The damage parameter can be written as ([14], see also [3]) with failure initiation at a critical damage parameter value of D_c . Here $\bar{\epsilon}_{pl}$ is the effective plastic strain, $\epsilon_{pl,c}$ the critical plastic strain, η the stress triaxiality, $\eta = \sigma_H/\sigma_v$, σ_H the hydrostatic stress, and σ_v is the von Mises equivalent stress. The damage parameter fulfils all demands on locality, triaxiality of the stress-strain field, as well as taking into account the complete failure history.

$$D = \int_0^{\epsilon_{pl,c}} e^{\frac{3\eta}{2}} d\bar{\epsilon}_{pl} \quad (2.11)$$

⁴ Reprinted from L. Mishnaevsky Jr., M. Dong, S. Hönle, S. Schmauder, "Computational mesomechanics of particle-reinforced composites", Computational Materials Science 16, pp. 133-143 (1999), with kind permission from Elsevier

The damage parameter (1) can be generalised in order to take into account the so-called “failure curves” of materials in the following way. Failure curves (see Fig. 2.22) present a relation between equivalent plastic strain and stress triaxiality at the crack initiation point inside the specimen, obtained on the basis of combined experimental and numerical investigations on tensile specimen ([15], see also [10]). The failure curve separates the equivalent plastic strain-stress triaxiality space into two parts. Below the curve the material is saved, no failure will occur. Points on the curve indicate failure initiation for a given stress-strain field. If one expresses the failure curves as shown in Fig. 2.22 as

$$\varepsilon_{pl,c} = A \cdot e^{-B\eta_c} \quad (2.12)$$

where A and B are two material-dependent parameters, and assuming that usually $\varepsilon_{pl} \leq \varepsilon_{pl,c}$ and $\eta \leq \eta_c$ holds during loading, one can derive the modified damage parameter [10]:

$$D = \frac{1}{A} \int_0^{\varepsilon_{pl,c}} e^{B\eta} d\tilde{\varepsilon}_{pl} \quad (2.13)$$

with the point of failure initiation at a critical damage parameter value of $D_c = 1$.

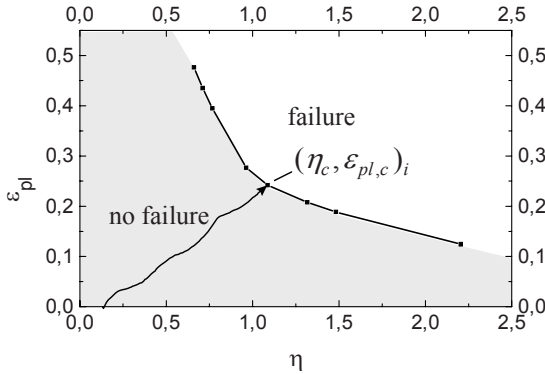


Fig 2.22 Scheme of a failure curve

Determination of the condition of element elimination: an example

To demonstrate how the condition of element elimination can be determined from experimental data, let us consider a simple macroscopical simulation of crack growth in Al/SiC (20 vol%) composites under 3-point-bending. An FE mesh similar

to the mesh given in [3] was taken in the simulation. However, a criterion of element elimination different from that used in [3] was applied: instead of the critical plastic strain, the Rice and Tracey's damage parameter was chosen as criterion for element elimination. The calculations were carried out for a material with averaged elastic properties of the specimen ($E = 99.4$ GPa and $\nu = 0.323$).

The difference between the critical plastic strain and Rice and Tracey's damage criterion for element elimination is determined by the fact that the Rice and Tracey's damage criterion is very sensitive to the degree of triaxiality in the deforming material, while this is not the case for the critical plastic strain criterion. The finite elements which are located on the loading surface were assumed to be elastic and were not subject to damage in order to simplify the simulation of the specimen/holder contact conditions. Based on the available data about the critical values of damage [3,7,9] we used three different values of critical damage parameters: $D_c = 0.5$, 0.15 and 0.2. As a result, the force-displacement curves for the specimen were obtained. The curves for the different values of the critical damage parameter are shown in Fig. 2.23. Although the peak points of the force-displacement curve were determined correctly and correspond to the experimental data, the appearance of the descending branch of the curve differs significantly from the experimentally observed results [3].

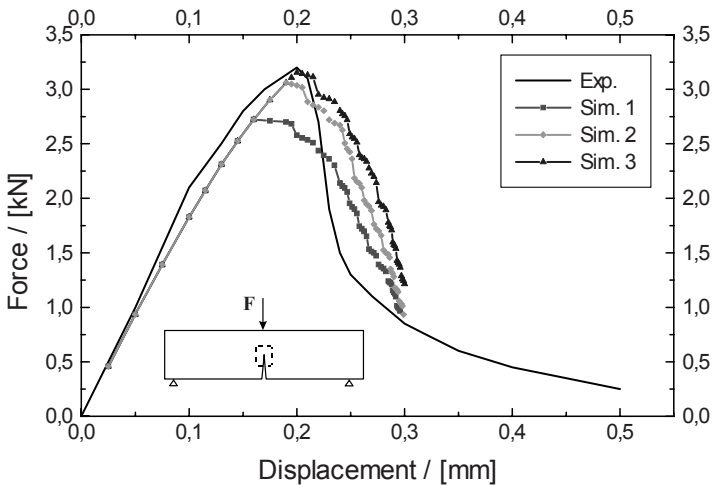


Fig 2.23 Force-displacement curves for 3-point bending. Sim.1 ($D_c = 0.2$), Sim. 2 ($D_c = 0.15$), Sim.3 ($D_c = 0.10$).

The values of the calculated peak load for the different critical damage parameters as well as the experimentally obtained peak load are given in table 2.3. It is found that the critical damage parameter $D_c = 0.2$ results in simulating the correct peak load. Therefore, our results confirm the data from [3,10], that the critical value of Rice and Tracey's damage parameter for Al/20 vol% SiC should be taken

as $D_c = 0.2$. The described procedure shows how the criterion of element elimination can be determined by comparing the experimental and numerical force-displacement curve.

Mesomechanical modelling of damage and failure in real structures

In this section, the model of damage initiation and growth, and fracture in a material with real structure is presented. In this model, both the multiphase element method and the EET are used. The simulation is carried out for WC/Co hard metals, which present particle-reinforced composites with coarse microstructure; these materials are characterised by a typically high content of hard inclusions and their relatively large size as compared with the thickness of areas of Co binder. A model microstructure of WC/Co material was taken and used in the simulations. The WC/Co specimen possesses a cobalt volume fraction of 16% and an average carbide size of $1.5 \mu\text{m}$.

The microstructure is meshed using multiphase elements (MPFEs) and is embedded in an environment with the elastic material behaviour of the composite and a pre-crack just in front of the real structure (Fig. 2.24).

The material properties of the carbide are elastic and the elastic-plastic behaviour of the cobalt is represented by a modified Voce-type flow law with an additional Hall-Petch term [10], according to where $\sigma_y = 270 \text{ MPa}$ - the yielding stress of cobalt, ($\sigma_s = 970 \text{ MPa}$, $\epsilon^* = 0.06$, $k_y = 7 \text{ N mm}^{-3/2}$ (material constants) and an average binder layer thickness of $L = 0.5 \mu\text{m}$ were taken from [16].

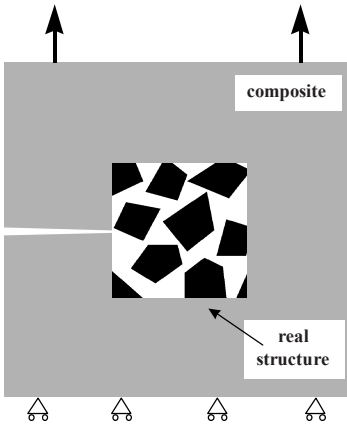


Fig 2.24 Micromechanical model for failure simulation in realistic structures.

Critical plastic strains and stress triaxialities, which were derived using crystal plasticity theory [17] at a critical void volume fraction of 15% [18] are shown in Fig. 2.22.

$$\sigma = \sigma_y + (\sigma_s - \sigma_y) \cdot \left[1 - \exp\left(-\frac{\epsilon}{\epsilon^*}\right) \right] + k_y L^{-1/2} \quad (2.14)$$

These results lead to the modified damage parameter,

$$D = \frac{1}{1.04} \int_0^{\varepsilon_{pl,c}} e^{1.12\eta} d\tilde{\varepsilon}_{pl} \quad (2.15)$$

In the following, results of a crack propagation simulation based on Eq. (2.15) are described. As a first attempt, a hard meta I with a high cobalt content and no contact between carbide particles was modelled and investigated under external tensile loading (see Fig. 2.25(a)). This study focused on the failure behaviour of the ductile cobalt phase. Brittle fracture in the carbide phase was thus suppressed. At the considered level, (mesolevel) the structure of material was practically random, and therefore, no special consideration of the texture dependence was required in this case. The results achieved on the level of crystal plasticity were calculated for a wide range of microscopic arrangements and crystallographic slip system arrangements, and thus describe an averaged behaviour of the material based on crystal plasticity theory.

Figs. 2.25(b)-(e) show crack initiation and crack propagation in this structure. The crack enters the real structure by initiating a void (Fig. 2.25(b)), which starts to grow under increasing load. Further increase of the applied load leads to void initiation in front of the crack tip (Figs. 2.25(c) and (d)) and coalescence with the main crack. Crack propagation is found to be a consequence of nucleation, growth and coalescence of the voids. This numerical study is in agreement with experimental findings on WC/ Co hard metals [19]. The force-displacement curve for this crack propagation depicts the experimental macroscopic failure behaviour of WC/Co hard metals as a quasi-brittle failure. The applied load increases nearly linearly, while it drops immediately when the critical load is reached.

Thus, local damage behaviour of the ductile cobalt phase is introduced in microscopic crack propagation simulations by making use of failure curves.

Table 2.3

Peak loads on the force-displacement curves at different critical values of Rice and Tracey's damage parameter

Critical damage parameter, D_c	0.1	0.15	0.2	Experiment [3]
Peak loads (kN)	2.76	2.95	3.1	3.1
Displacement (mm)	0.22	0.24	0.26	0.2

Meso-macromechanical modelling of damage and failure of two-phase composites

Microdamage in Al/Si cast alloys: unit cell simulation

In Al/Si cast alloy specimens, the damage process is determined by the strength of Si-particles and the Al matrix as well as the shape, size, arrangement and volume fraction of the Si-particles.

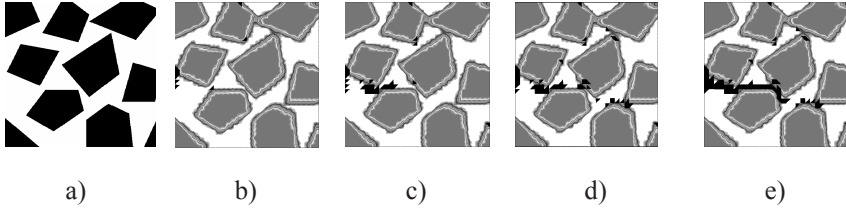


Fig 2.25 (a) Idealised real structure (WC black, Co white), (b)-(e) void nucleation, growth and coalescence.

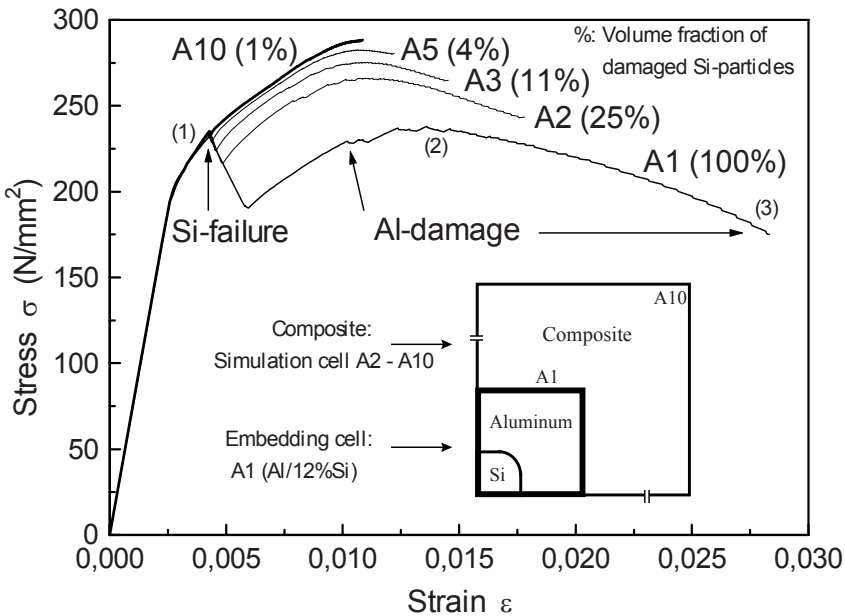


Fig 2.26 Local stress-strain relations of the Al/12%Si cast alloy concerning both particle cracking and matrix failure for different volume fractions of locally damaged material.

The Si-particles behave elastically and the Al-matrix elasto-plastically. It is known that only large Si-particles fracture during external loading [8,9]. Large particles are present at a low volume fraction of about 1-5% in the alloy, while the overall volume fraction of Si amounts to 12%.

In the mesomechanical model, a unit cell containing a silicon particle and the aluminum matrix is embedded in an equivalent homogeneous material with the same mechanical behaviour as that of the embedded cell (Fig. 2.26). Under the tensile displacement loading of the upper external boundary of the embedding composite in the cell shown in Fig. 2.26, the overall response of the inner embedded cell is obtained by averaging the stresses and strains in the embedded cell [20].

Microdamage of the two-phase material in the embedded cell [20] is simulated by a hybrid local approach for brittle cracking of silicon particles and for ductile failure of the aluminum matrix (Figs. 2.26 and 2.27). The normal stress criterion ($\sigma_{\max}^n = 320 \text{ Mpa}$) obtained from comparison of simulation and experiment in [21]) and node release technique are applied to simulate Si-particle cracking whereas the damage parameter D and the EET are applied for simulating ductile void growth in the Al-matrix. The damage parameter involves the loading state as well as the loading history and its critical value can be derived from the corresponding experiment and simulation (in this case, $D_c = 0.7$ [22]).

At a total strain of $\epsilon_{\text{tot}} = 0.43\%$ the Si-particle is cracking orthogonally with respect to the tensile loading direction according to the normal stress criterion and then matrix damage occurs subsequently under increasing loading. The matrix damage propagates in the same direction as the Si particle crack. Local stress-strain relations of the Al/12% Si cast alloy concerning both particle failure and matrix damage are thus obtained for different volume fractions of locally damaged material (Fig. 2.26), which are further taken into account in the macromechanical model.

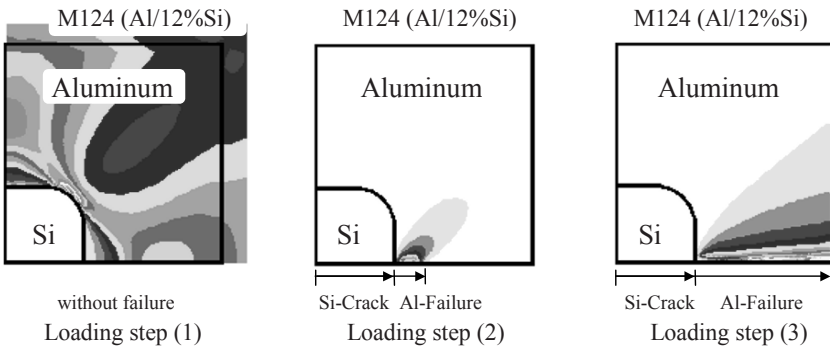


Fig 2.27 Local damage parameter distribution in the embedded cell for three different loading steps according to Fig. 2.26. White areas: $D = 0$, very bright areas: $D = 0.6 \dots 0.7$, dark areas: $D = 0.4 \dots 0.5$, medium dark till areas: $D = 0.1 \dots 0.3$.

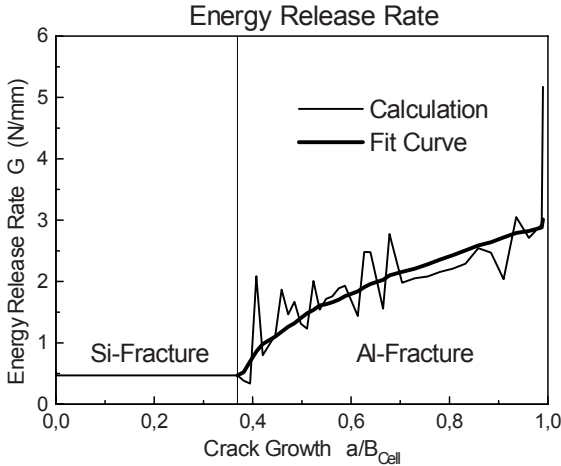


Fig 2.28 Energy release rate of matrix damage after silicon particle cracking

The local damage-parameter distribution in the embedded cell for the three different loading steps (Fig. 2.27) shows the development of damage-parameter concentration, which results in void growth and crack propagation in the matrix. The released energy is an important magnitude for comparison with the non-destructive evaluation of damage by acoustic emission.

From local energy considerations, the energy release rate by further damage propagation can be calculated as a function of microcrack length (Fig. 2.28). After fracture of the silicon particle, the energy release rate of the matrix damage increases with sub-critical microcrack growth until rupture of the material.

Macromechanical model of failure in Al/Si cast alloys

On the basis of the above-described mesomechanical model, macromechanical models of tensile or compressive specimens are set up to investigate crack growth. The mechanical behaviour of the Al/12%Si cast alloy with damage evolution was assigned to each finite element taking into account damage initiation and propagation calculated from the mesomechanical models presented above. In this way, the macroscopical development of microdamages until rupture of the specimen can be simulated. As an example, an initial Si-failure is introduced at a corner of a homogeneous specimen. The propagation of Si failure is calculated according to the critical normal stress obtained from micromodelling.

The simulations demonstrate two stages of damage evolution: At first the Si-particles fail along shear bands which nucleate from the initial failure side in the specimen at the macroscopic plastic flow stage, as shown in the stress distribution in Fig. 2.29. After Si-failure, the specimen can still carry increased loading and stretching.

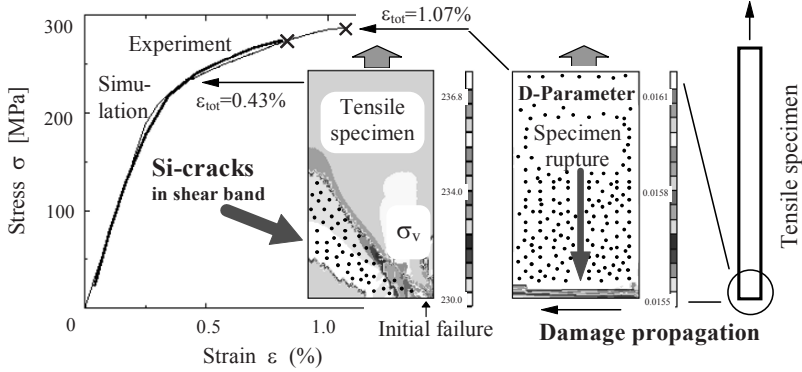


Fig 2.29 Macroscopical development of microdamages at different loading stages (areas of cracked Si-particles are represented by black dots).

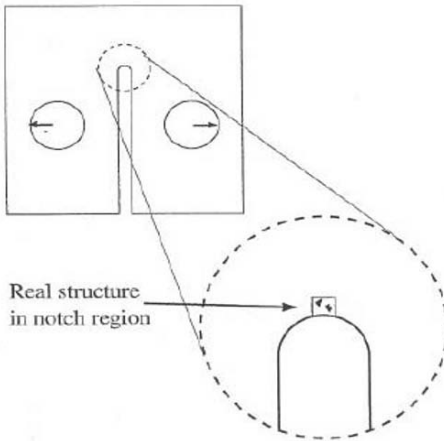


Fig 2.30 Scheme of loading of CT specimen and location of the area with real microstructure.

Under further loading, the damage parameter concentration increases in the cross section orthogonally to the loading direction and the crack starts to propagate perpendicular to the loading direction until failure of the specimen in agreement with the observations of fracture in such materials [20] (Fig. 2.29)

3D FE-simulation of deformation in real structures

In this section, the results obtained by Mishnaevsky Jr. et al. [6] in the framework of the COST -Project “Microstructural investigation of failure mechanisms in Al/Si cast alloys by 3D FE modelling” are reported and compared with

above-described 2D models of mechanical behaviour of composites. To simulate the deformation of specimens from Al/Si cast alloys with different microstructures, 3D MPFE has been applied.

The small volume in which the real structure was reconstructed is located in the notch region of loaded compact tension (CT) specimen. The scheme of loading CT specimen is shown in Fig. 2.30. For a small volume ($100\text{ }\mu\text{m} \times 100\text{ }\mu\text{m}$) in the notch ground region the microstructure of material was reconstructed with the use of digitised micrographs of polished sections as described above. The properties of components (Al-matrix and Si-particles) have been assigned to finite elements in correspondence with distribution of “black” and “white” areas on digitised micrographs.

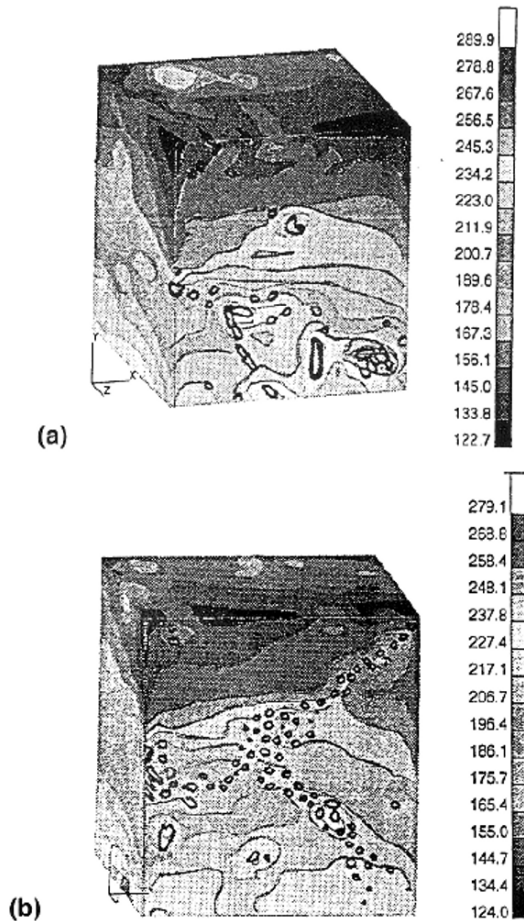


Fig 2.31 Stress distribution (σ_v) in the regions with real microstructure: (a) lamellar; (b) globular microstructure. Only particles at the surface are shown (for details see text).

The rest of the specimen was assigned the averaged properties of Al/Si cast alloy. In the area of real microstructure, there were 4000 finite elements, in the full specimen 16000 FE. The simulation was carried out for two alloys: one with lamellar and one with globular microstructures. The load was increased in five loading steps, each was 100 N. The mechanical properties and stress strain curve of Al-matrix and Si-particles have been determined experimentally as described in [6].

Some results of the simulation are shown in Fig. 2.31: the von Mises stress distribution in the region with real structure for both types of the alloy microstructure. The von Mises stress distribution is presented in order to study the effect of Si-particles on the stress field in the material. From Fig. 2.31 one can see that the Si-particles cause high local stress concentrations, especially on the notch surface. One may suppose that the high local stress concentrations lead to damage initiation in the vicinity of Si-particles. The experimental investigations of damage evolution in Al/Si cast alloys [6, 21, 23] confirm this assumption: microcracks have been formed in the vicinity of Si-particles, often near the notch surface, and then grow and form large cracks.

The developed approach permits 3D FE-simulations of deformation and local effects in heterogeneous materials, using the reconstructed real structures and the method of multiphase elements. However, the accuracy of 3D simulation depends strongly on the degree of fineness of the FE mesh and on the amount and quality of layers (sections) from which the 3D real structure is reconstructed. For both factors, there are unavoidable limitations (computational and experimental, respectively), which limit the possibility of this model.

Conclusions

In this paper, the results of application of advanced numerical methods (MPFE and EET) for the simulation of the mechanical behaviour and failure of particle-reinforced composites were presented.

Several aspects of FE simulation of particle-reinforced composites were considered:

- method of determination of conditions of local failure;
- modelling of deformation and fracture in coarse particle-reinforced composites (WC/Co hard metals, in this case);
- multilevel modelling of deformation and fracture of composites with fine particles; transition from a mesomechanical model of behaviour of composites with relatively fine particles (Al/Si) to the macroscopical model of material;
- possibility of generalisation of 2D methods of FE simulation of materials with real structures to the 3D case.

The methods are applied to model the mechanical behaviour of different types of materials: quasi-homogeneous (macromodels of Al/Si and Al/SiC), coarse particle-reinforced composites (WC/Co hard metals) and fine particle-reinforced composites with different types of microstructures (lamellar, globular) (Al/Si).

A mesomechanical model of damage and fracture of hard metals made it possible to determine the mechanisms of fracture. It is shown numerically that crack propagation can be simulated as a result of nucleation, growth and coalescence of voids. The force-displacement curve for this crack propagation depicts the experimental macroscopic failure behaviour of WC/Co hard metals as a quasi-brittle failure: the applied load increases nearly linearly, while it drops immediately when a critical load is reached. The local damage behaviour of ductile cobalt phase in hard metals was taken into account in the simulations by using the failure curves.

The possibility of generalisation of the FE model of the mechanical behaviour of material for the 3D case has been explored. Although there are some essential limitations in the used experimental and numerical techniques, related with the difficulties of obtaining many micrographs of sections of a material volume with strictly equal distances between them, and the limited amount of elements in the mesh, which must be however very fine, this first trial of 3D simulation of deformation of real structures has demonstrated possibilities of this approach.

Although the purely one-scale level models are appropriate for solving some partial problems (like the quasi-homogeneous model for the determination of the condition of element elimination in the material with low-filler content, and the mesomodel for the simulation of coarse composites like hard metals), the multi-level approach seems to be more promising, and can allow to describe the behaviour of material taking into account real physical mechanisms of material behaviour.

Thus, the meso-macromechanical model allows simulating the damage evolution and failure in an Al/Si alloy. The mechanism of failure of the alloy has been clarified. It has been shown numerically, that the failure of a large Si-particle causes subsequent damage of the Al-matrix on the microlevel. It is found that Si-particle cracking takes place at much higher loading levels in compression than in tension and no further Al-matrix damage occurs. After cracking of the Si-particle, the material can be further loaded. Sub-critical crack growth induces plastic deformation in the matrix. Si-particles fail in macroscopic shear bands which are initiated at crack tips before ductile rupture of the specimen in the main crack plane perpendicular to the loading direction.

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2.3 Automatic generation of 3D microstructure-based finite element models

2.3.1 Idealized microstructures of particle reinforced composites: multiparticle unit cells with spherical inclusions⁵

Numerical simulations of deformation, damage and fracture of composites present an important tool for the prediction of materials behavior, and the optimization of mechanical properties of materials. In most cases, such numerical simulations are carried out two-dimensionally [1]. However, it has been shown in several works that results of 2D approximations are generally not correct for 3D case [1–5,9]. So, Jung et al. [5] compared results (stress and strain distributions) of the 2D and 3D FE simulations, and found that a 2D approximation gives results which are sufficiently different from the 3D solution. Therefore, the necessity of using three-dimensional simulation methods to analyze three-dimensional problems becomes apparent.

Several methods and concepts of FE simulation of deformation and damage of multiphase materials taking into account their microstructure have been developed in last years. table 2.4 gives a short overview of these methods. One can see from the table, that the mesh design for complex 3D microstructures and incorporating the microstructure data into FE models are one of main challenges of the 3D numerical testing and design of materials, which is met by using different techniques (multiphase finite elements, hierarchical models, Voronoi cell finite elements, etc.).

The purpose of this work was to develop a simple and efficient method of automated microstructure generation and mesh design, and to carry out systematic numerical testing of microstructures of composites. To simplify and automate the design of meshes for the 3D virtual testing of microstructures, a program “Meso3D” was developed. The program works with the commercial software MSC/PATRAN and produces artificial microstructures (i.e., different arrangements of round and ellipsoidal inclusions in a matrix) on the basis of given parameters and probability distributions of particle coordinates and sizes, and generates databases for the computational (finite element) testing of the materials with the required artificial microstructures. The designed microstructures are meshed with tetrahedral elements using the free meshing technique [27].

The microstructures with the random particles arrangement were generated using the uniform random number generator. Each coordinate was produced independently, with another random number seed. After the coordinates of a first particle were defined, the coordinates of each new particle were determined both by using the random number generator, and from the condition that the distance

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between the new particle and all available particles is no less than 0.1 of the given particle radius. If the condition was not met, the seed of the random number generator was changed, and the coordinates of the new particle were determined anew. In order to avoid the boundary effects, the distance between a particle and borders of the box was required to be no less than 0.05 particle radius. The coordinates of the centers of particles for the regular (and any other pre-defined) particles arrangements are read from a text input file.

Table 2.4

Some 3D approaches to the micromechanical modelling of materials

Approach	Examples and peculiarities of the approaches
Unit cell with a single inclusion	Classical approach, based on the assumption that the local behavior of the material follows a periodic pattern
Unit cells with many inclusions	The multiparticle unit cell model (see [2–4, 6, 7]) allows a simple generalization of conclusions obtained with the unit cells on the whole specimen. The simulations can require rather high computational resources
Hierarchical models	Example: a “super-element” approach developed by Geni and Kikuchi [8]. In the framework of this approach, a composite is modeled with a box-shaped super element, consisting of many different cylindrical unit cells with different particle volume fraction and shapes of particles
Voronoi cell finite element models (VCFEM)	FE mesh is created by Dirichlet tessellation. Each polygon, formed by such tessellation (“Voronoi cell”) contains one inclusion at most and is used as a finite element. In the 3D version, the microstructures of composites are “reconstructed by assembling digitally acquired micrographs obtained by serial sectioning”. 3D equivalent microstructures (with real particles replaced by ellipsoids) are tessellated into a mesh of Voronoi cells, and the deformation and damage in these equivalent structures are simulated [9–11]
3D multiphase finite element method (MPFE) for real structure simulations	A 3D real microstructure of a material is included into a FE model by assigning the phase properties to the integration points according to the digitized images of microstructures [13,14]. The microstructure of the material is reconstructed using the image

analysis of micrographs of many sections (cuts) of materials

Design of materials on the basis of virtual testing and the statistical genetic algorithm

In the framework of the approach, developed by Zohdi et al. [15–17], large-scale micromechanical simulations are carried out by decomposing the global domain into a set of computationally smaller, decoupled problems, which deal with subdomains of the global domain. Microstructures of the materials are included into the numerical models of the subdomains on the basis of the Gauss point method. The optimal shape of inclusions was determined numerically using the statistical genetic algorithm

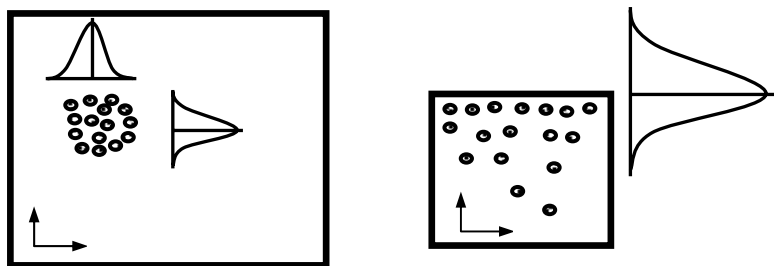


Fig. 2.32 Schema of the design of clustered (a) and gradient (b) microstructures.

In order to generate the localized particle arrangements, like clustered, layered and gradient particle arrangements, the coordinates of the particle centers were calculated as random values distributed by the Gauss law. The mean values of the corresponding normal distribution of the coordinates of particle centers were assumed to be the coordinates of a center of a cluster (for the clustered structure), or the Y- or Z-coordinate of the border of the box (for the gradient microstructure). Fig. 2.32 shows schematically examples of such a design of the microstructures. The standard deviations of the distribution can be varied, from highly clustered or highly gradient arrangements (very small deviation) to the fast uniformly random particle arrangements (a deviation comparable with the box size).

Finite element simulations and results

FE model, damage mechanisms and properties of phases

The problem was solved in the framework of the embedded cell approach [1, 26]. The main idea of the embedded cell approach is that microfields in inhomogeneous materials are determined, using a model consisting of a core (“local heterogeneous region”), embedded in an outer region that serves mainly for introducing loads into the core and has the averaged properties of the composite [13, 26]. According to Böhm [26], this strategy “avoids some of the drawbacks of the periodic field approach, especially the requirement that the geometry and all microfields must be strictly periodic”. Then, the embedding allows avoiding the boundary effects on the particle failure. In our case, the FE meshes of the composites with different microstructures (a given amount of SiC particles in a box 10x10x10 mm, filled with elastoplastic Al matrix), generated with the use of the program “Meso3D” and commercial code MSC/PATRAN, were placed in a bigger box 14x14x14 mm. The embedding zone behaved as a composite with averaged properties, i.e., as an elastic–plastic material (Al/10%SiC).

The SiC particles behaved as elastic isotropic damageable solids, characterized by Young modulus $E_p = 485$ GPa, Poisson’s ratio 0.165 and the local damage criterion, discussed below. The Al matrix was modeled as isotropic elasto-plastic solid, with Young modulus $E_M = 73$ GPa, and Poisson’s ratio 0.345. The experimental stress–strain curve for the Al matrix was taken from [28]. The elements in the embedding were assigned the averaged mechanical properties of the Al/ SiC composite, with Young modulus $E_{Av} = 75.7$ GPa (for the volume content 10%) and $E_{Av} = 88.4$ GPa (for 15%), and Poisson’s ratio 0.323 taken from [12, 13, 24]. The elasto-plastic stress–strain curve for the composite (embedding) was taken from [12] as well. The experimental stress–strain curve for the matrix as well as the constitutive law for the composite (embedding), taken from [12] were approximated by the deformation theory flow relation (Ludwik hardening law): $\sigma_y = \sigma + h\varepsilon_{pl}$ where σ_y – the actual flow stress, σ_{yn} – the initial yield stress, and ε_{pl} the accumulated equivalent plastic strain, h and n – hardening coefficient and the hardening exponent. The parameters of the curve for the matrix were as follows: $\sigma_{yn} = 205$ MPa, $h = 457$ MPa, $n = 0.20$. For the composite (embedding), the parameters were: $\sigma_{yn} = 216$ MPa, $h = 525.4$ MPa, $n = 0.25$.

The nodes at the upper surface of the box were connected, and the displacement was applied to only one node. The model was subject to the uniaxial tensile displacement loading, 2.0 mm.

We considered cells with 5, 10 and 15 particles, the volume content of the inclusion phase was 2.5%, 5%, 10% and 15%. Totally, the models contained about 30,000 elements. Each particle contained about 400 finite elements. The radii of particles were calculated from the prescribed volume content and particle amount in the box, and were as follows: 1.1676 mm (volume content/ VC = 10%, N =

15), 0.9267 mm (VC = 5%, N = 15), 1.3365 mm (VC = 10%, N = 10) and 1.0608 mm (VC = 5%, N = 10).

The uniaxial tensile response of each microstructure was computed by the finite element method. The simulations were done with ABAQUS/Standard.

The damage was modelled as a local weakening of a finite element in which the damage criterion (maximum principal stress) exceeded a critical value. An ABAQUS Subroutine USRFLD, which allows simulating the local damage growth as a weakening of finite elements was developed. After an element failed, the Young modulus of this element was set to a very low value (50 Pa, i.e., about 0.00001% of the initial value). Only the elements in which the maximum principal stress exceeded a critical value (and not all the elements in the particle) were weakened in the framework of this algorithm [18–20].

Baptiste [21], Hu et al. [22] and Derrien et al. [23] have demonstrated that the main mechanism of damage initiation for the AlSiCp systems is the particle failure. According to Derrien and co-workers [23, 24], the failure of specimen occurs by linking of the microcracks initiated in the matrix from the broken particles. In the matrix near the broken particle, the cavities and microvoids nucleate, grow and coalesce, and that leads to the failure of the matrix ligaments between particles. A similar result was obtained by Kobayashi et al. [25]: „since the interfacial bonding strength is sufficiently high in the case of an Al/SiC system, the predominant factor for toughening is the fracture strength of reinforcements”. Therefore, only damage in SiC particles was considered at this stage of the work. According to [21–23], the SiC particles in AlSiC composites become damaged and ultimately fail, when the critical maximum principal stress in the particle material exceeds 1500 MPa. This value was used in our simulations as a criterion of damage of SiC particles as well. As output parameters of the numerical testing of the microstructures, the effective response of the materials and the amount of failed particles NF versus the far-field strain curves were considered. The displacement loads, at which the first particle fails and at which most particles fail, as well as the rate of failure of particles (determined as a slope of the NF– ϵ curve in its linear part) were considered as parameters of the damage growth rate in the materials, which depend on their microstructures. To characterize the “rate of particles failure” v_F quantitatively, we calculated it as the total amount of failed particles in the cell divided by the displacement difference between the point where the first particle failed ($u_{1st_particle_fail}$) and the last particle failed ($u_{all_particles_fail}$).

The generation of a microstructure and pre-processing for each cell took about 15 min (2–3 min of this time were interactive) on the Compaq personal computer and 2 GB of RAM. The analysis of a model took about 10 h on the SERVus cluster of the University of Stuttgart.

Deformation and damage behavior of composites with the random arrangement of particles

The deformation and damage evolution of the Al/SiC composites with random SiC particle arrangements were simulated with the use of the above described model. The purpose of this part of the investigation was to verify whether the “random” particle arrangements have peculiarities as compared with regular or localized particle arrangements, and whether these peculiarities are stable, reproducible and typical for the random arrangements.

Since the random particle arrangements were generated from a pre-defined random number seed parameter (idum), (which should ensure reproducibility of the simulations), variations of this parameter lead to the generation of new microstructures. Five realizations of the random microstructures with 15 spherical particles and volume content of ceramic phase 10% (produced with different random numbers seeds) were generated and tested.

Fig. 2.34(a) shows the tensile stress–strain curves for the five random arrangements (15 particles, volume content 10%). For comparison, we included also the curves for the regular and gradient particle arrangements. Fig. 2.34(b) gives the amount of failed particles plotted versus the far-field applied strain. Fig. 2.33 shows the equivalent plastic strain in a cell with randomly arranged 10 particles (VC = 5% and 10%) both on the boundaries of the box and on the matrix/particle interfaces.

One can see from Fig. 2.34, that the effective responses of the materials with random microstructures (even in different realizations) lay very close one to another and differ from that for the regular or localized microstructures. However, some variations of both flow stress and damage behavior of different random microstructures are observed as well, especially, after the far-field strain exceeds 0.1. The difference between the stresses for different realizations of the same random structure falls in the range of 2% even at the rather high far-field strain ($\varepsilon = 0.2$). For comparison, the difference between the regular and gradient particle arrangement is about 16% at the far-field strain 0.2, and 9% at the far-field strain 0.1 (see Fig. 2.39). Therefore, although the stress–strain curves diverge a little bit when the strain is higher than 0.1, the differences between realizations of the random microstructure are still much smaller, than the difference of the mechanical response between the different types of the microstructures.

In the following parts, at least three to five realizations of random microstructures will be simulated and averaged, when a random microstructure is compared with other microstructures. The rate of particle failure is lower for all the considered random particle arrangements than for the regular and clustered microstructures: the fraction of failed particles increases from 40% to 80%, when the far-field strain increases 2.8 times in the case of the random particle arrangement, and increases from 20% to 86% when the far-field strain increases 1.5 times for the regular particle arrangement.

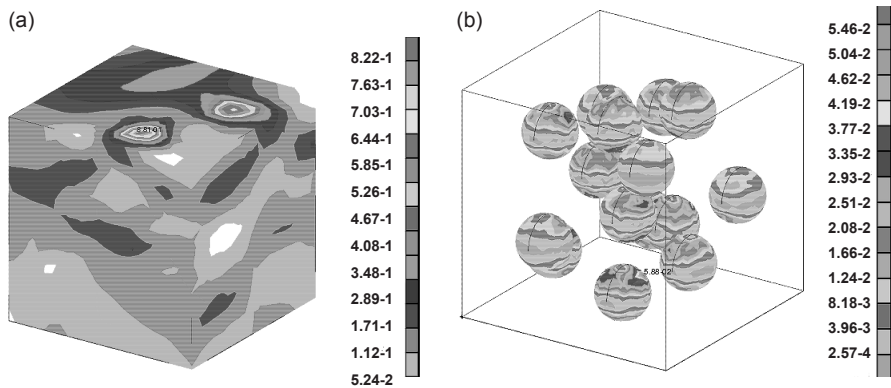


Fig. 2.33 Equivalent plastic strain in a cell with randomly arranged 10 particles: whole unit cell (a) and on the matrix/particle interfaces (b). VC = 10%. Total strain = 0.25.

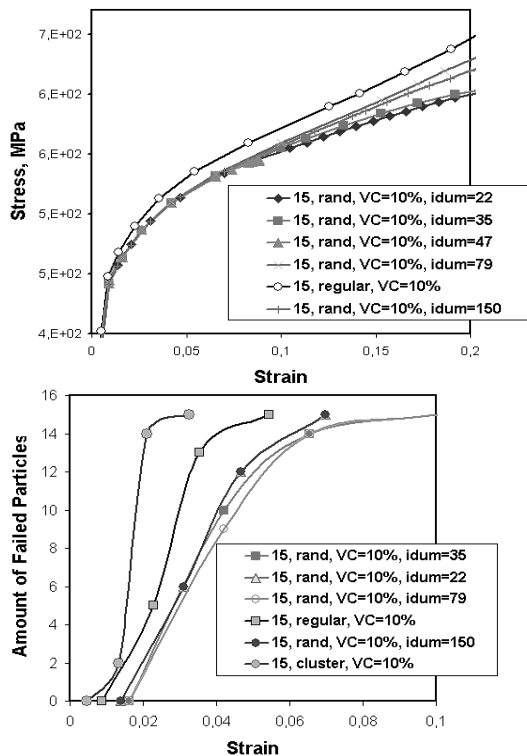


Fig. 2.34 Stress-strain curves (a) and the amount of failed particles plotted versus the far field strain (b) for the five random arrangements (15 particles, VC = 10%) and for the regular particle arrangement.

One can see that the flow stress for the regular microstructure of the composite is higher than that for the random microstructures (in the following paragraphs, we could see that the regular microstructure ensures highest flow stress among all considered microstructures). It is of interest that in the simulations by Segurado et al. [7] the flow stress for the regular BCC particle arrangement was significantly lower than for the random particle arrangement. The difference between our result and the results by Segurado et al. [7] can be caused by the fact that the model from [7] does not take into account the stress redistribution in the composite due to the reinforcement fracture. The varied distance between particles together with the effect of the interaction of cracks in neighboring particles in the case of the random particle arrangement can lead to the formation of weakened regions with high density of failed particles. The deformation of the weakened regions determines the low stiffness of the whole cell. This is not the case if the particles are placed equidistantly, as in the regular microstructures, and the local weakening in a particle is averaged over the entire specimen. Therefore, the constant large distance between particles, typical for the regular microstructures, can prevent the formation of weakened areas in our case, but not in the model by Segurado et al. [7].

Effect of the amount of particles and the volume content on the deformation and damage in the composite

At this stage of the work, the effects of volume content of hard phase and the amount of particles on the effective response and damage behavior of the composite were considered.

Fig. 2.35 shows the tensile stress–strain curves for the random particle arrangements with varied amount of particle (volume content of particles 5%, amount of particles 5, 10 and 15, Fig. 2.35(a) and the same for the volume content 10%, Fig. 2.35(b)). Fig. 2.36 gives the tensile stress–strain curves for the regular particle arrangement with varied volume content of particles (10 particles, volume content varied from 2.5% to 15%, Fig. 2.36(a), and 15 particles, volume content was varied from 5% to 15%, Fig. 2.36(b)). Fig. 2.37 shows the amount of failed particles in the box plotted versus the far-field applied strain (10 particles, varied volume content, Fig. 2.37(a) and 15 particles, varied volume content, Fig. 2.37(b)).

One can see from Fig. 2.36 that the flow stress of composite increases with increasing the volume content of particles. An increase in the volume content by 5% leads to the increase of the flow stress by 4%, both for the cells with 10 and 15 particles.

The amount of particles (at the same volume content) influences the effective response of the material only at rather high stage of particle failure, when many particles failed already. In this case, the difference between the response of the composite with 5, 10 and 15 particles increases with increasing load, and the flow stress is higher for a composite with a higher amount of particles.

The curves of the amount of failed particles plotted versus the applied strain have an (almost) linear part (up to 10–12 particles of 15 fail) and an “asymptotic” part (when the amount of failed particles slowly approaches the total amount of

particles). Since the last part of the curve (“asymptotic”) hardly reflects the real damage growth process, one may define a “critical applied strain” as a far-field applied strain at which the linear part of the curve goes into the „asymptotic“ part of the curve. In most cases, this takes place when 80% of particles (12 particles of 15, or 8 particles of 10) fails.

The critical applied strain depends on the volume content of particles as well. One can see from Figs. 2.37(a) and (b) that the higher the volume content of particles, the lower is the critical applied strain. An increase of the volume content of particles by 5% leads to the decrease of the critical applied strain by 4; . . . ; 5%, both for the cells with 10 and 15 particles.

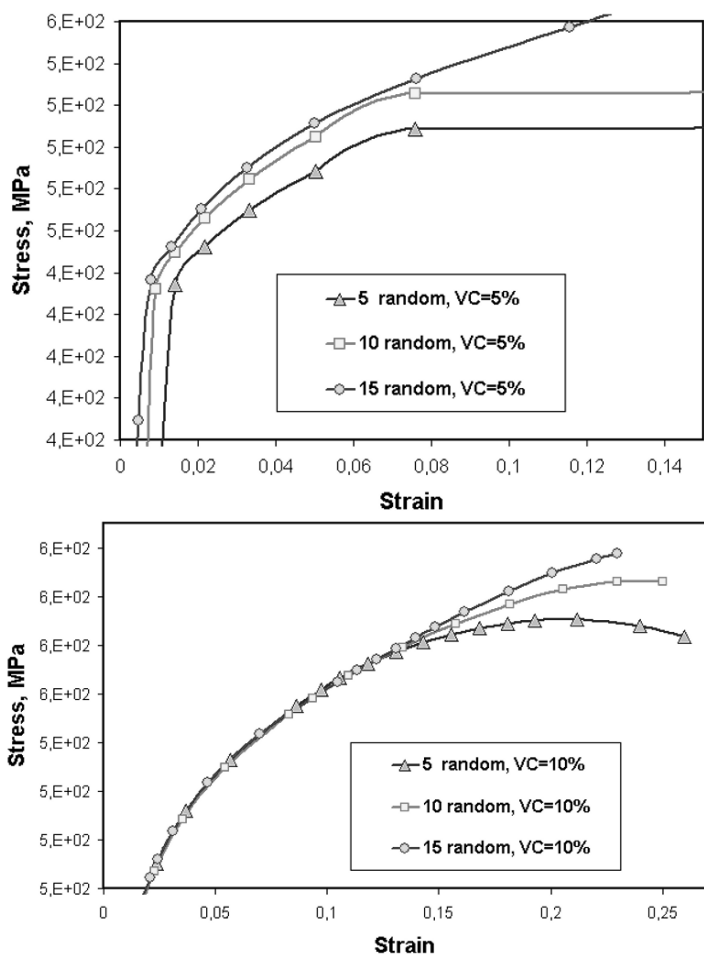


Fig 2.35 Stress–strain curves for the random particle arrangement, VC = 5% (a) and 10%, (b), amount of particles 5, 10 and 1

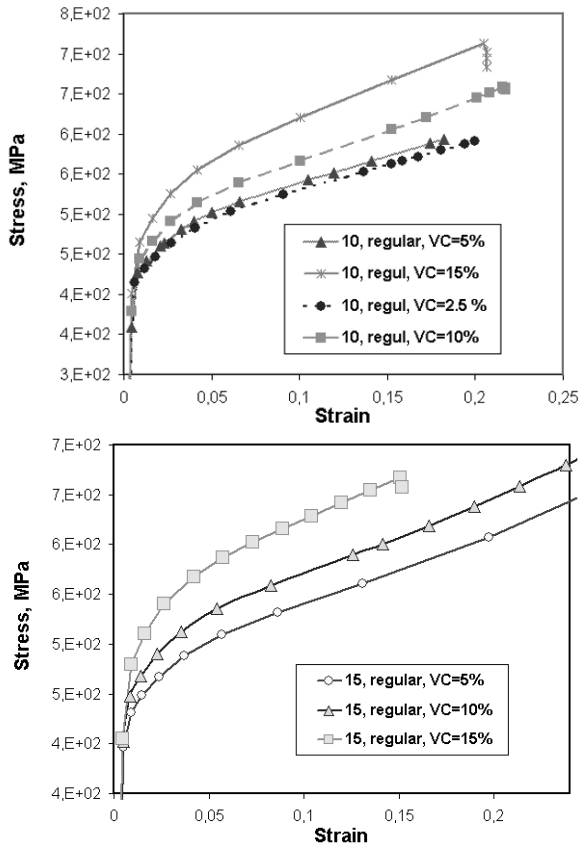
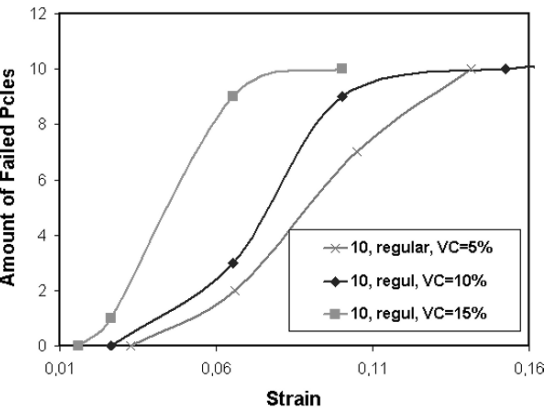


Fig. 2.36 Stress–strain curves for the regular particle arrangement: (a) 10 particles, and (b) 15 particles, volume content was varied.



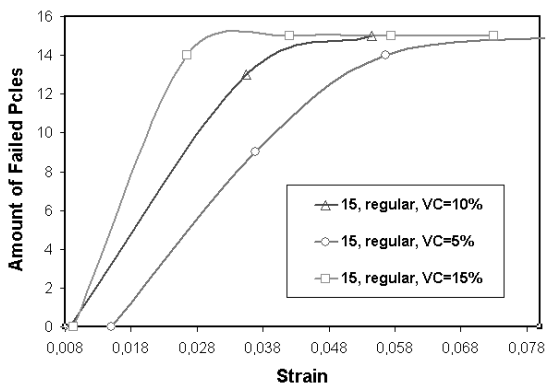


Fig. 2.37 Amount of failed particles in the box plotted versus the far-field applied strain: (a) cells with 10 particles; (b) 15 particles (varied volume content).

Effect of the clustering and gradient distribution of particles

At this stage of the work, the effects of particles arrangement and localization on the deformation and damage evolution in the composite were considered.

Fig. 2.38 shows the random (a), regular (b), clustered (c), and highly gradient (d) arrangements of the particles. Two types of the gradient particle arrangements were considered: an arrangement of particle with the vector of gradient (from low particle concentration region to a high particle concentration region) coinciding with the loading direction (called in the following a “gradient Y” microstructure), and a microstructure with the gradient vector perpendicular to the loading vector (called in the following “gradient Z” microstructure). The standard deviations of the normal distribution of the Y or Z coordinates of the particle centers (for the Y and Z gradient microstructures, respectively) were taken 2 mm, what ensured rather high degree of gradient. The same standard deviations were taken for the clustered particle arrangements. Fig. 2.39 shows the tensile stress–strain curves for the random, regular and gradient microstructures (for 10 particles, volume content of SiC 5%, Fig. 2.39(a)) and for the random, regular, clustered and gradient microstructures (for 15 particles, volume content of SiC 5% and 10%, Fig. 2.39(b)–(d)). Fig. 2.40 shows the amount of failed particles in the box plotted versus the far-field applied strain, for the same microstructures (15 particles, volume content of SiC 5% and 10%). The error bars show the deviations of the stress and the amount of failed particles from averaged values in 3–5 simulations. The deviations fall in the range of 2% for the random microstructures, and are even less for the gradient and clustered microstructures (0.5–0.9%).

It can be seen from Fig. 2.39, that the particle arrangement hardly influences the effective response of the material in elastic area or at small plastic deformation. The influence of the type of particle arrangement on the effective response of the material becomes significant only at the load at which the particles begin to

fail (compare the Figs. 2.39 and 2.40). However, after the particle failure begins, the effect of particle arrangement increases with increasing the applied load. (One should note here the difference with the case when only amount of particles and neither their content nor arrangement vary: in this case, the difference becomes sufficiently large only when most particles fail, see Fig. 2.35; in the case of the different particle arrangements, the influence of the arrangement becomes strong when a first particle fail already.)

After the first particle fail, the flow stress of the composite and the strain hardening coefficient increase with varying the particle arrangement in the following order: gradient < random < clustered < regular microstructure (see Fig. 2.39).

In order to analyze the effect of particle arrangement on the strain hardening quantitatively, we determined the stress hardening coefficients for the stress–strain curves shown in Fig. 2.39(c) and (d). The strain hardening coefficients were calculated as the power in the power like equation for the true stress–true strain curves, using regression analysis. Table 2.5 shows the strain hardening coefficients n for all the considered curves. For all levels of the volume content, the particle failure rate for 2.3 times higher for the cells with 15 particles, than for the cells with 10 particles: 18; . . . ; 29 particle/mm (for the cell with 15 particles and regular particle arrangement) and 45; . . . ; 90 particle/mm (for the cell with 10 particles).

One can see from figure that the critical applied strain decreases in the following order: gradient (10%) > gradient (5%) > random (5%) > regular (5%), random (10%) > cluster (5%) and regular (10%) > clustered (10%) (the volume contents of the SiC phase are given in brackets).

The strength and damage resistance of a composite with a gradient microstructure strongly depends on the orientation of the gradient in relation to the direction of loading. In the case of the “gradient Y” microstructure, the rate of particle failure is very low (about 6.35 particle/mm) and the particle failure begins at relatively high displacement loading, 0.2 mm. In the case of the “gradient Z” microstructure, the rate of particle failure is the same as for random microstructures. One should note that the highly gradient distributions of particles, considered here, constitute just one snapshot of many possible arrangements. Apparently, if the arrangement of particles changes from the highly gradient arrangement, considered here, to the arrangements with more slow gradients, the properties of the material will be changed. This will be the subject of further investigations.

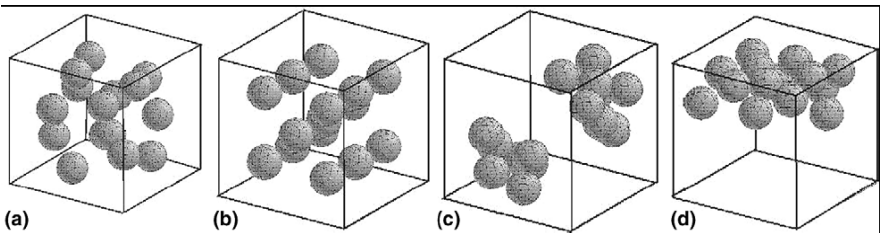
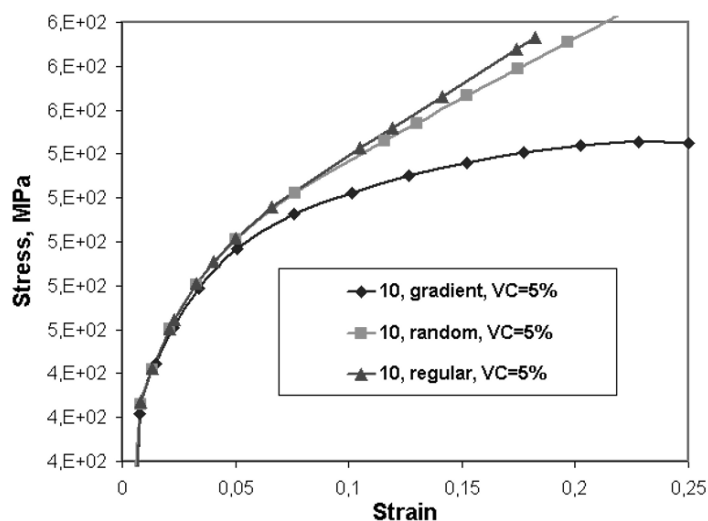
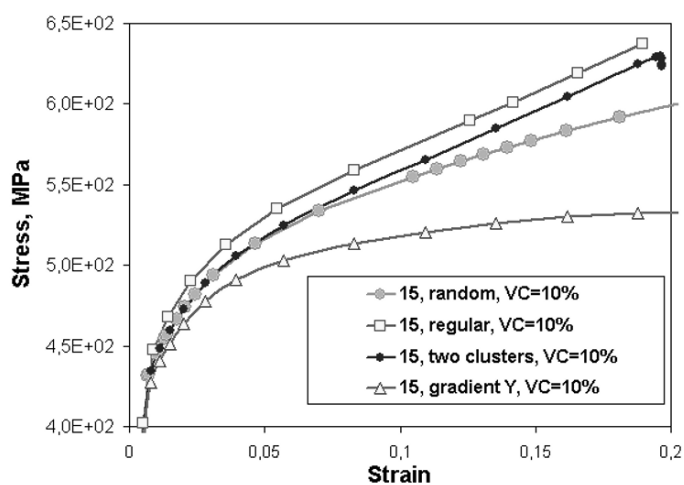


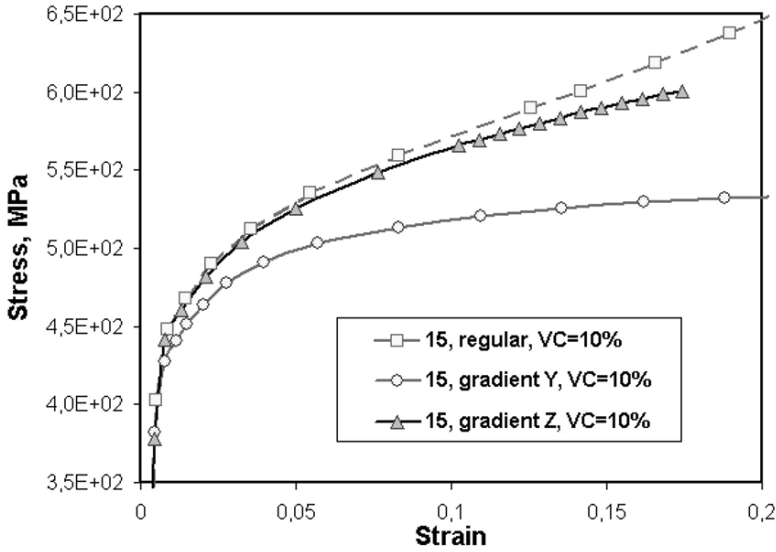
Fig. 2.38 Random (a), regular (b), clustered (c) and highly gradient (d) arrangements of the particles.



(a)



(b)



(c)

Fig. 2.39 Stress-strain curves for the unit cells with different particle arrangements: (a) 10 particles, VC=5%, (b, c) 15 particles, VC=10% microstructures

To characterize quantitatively the arrangements of particles and the degree of localization in different microstructures, we determined the nearest neighbor distances between the particle centers (NND), the nearest-neighbor index (NNI, ratio of observed to expected nearest-neighbor distance) and the statistical entropy of the nearest neighbor distance (SENND). The accurate determination of these parameters requires a much larger of particles than those generated to compute the mechanical behavior [7] and those considered in the unit cells above. To overcome this limitation, we followed the idea by Segurado et al. [7] who generated much larger unit cells, than those used in their numerical experiments, using the same algorithms, and determined the statistical parameters of microstructures with the use of the larger cells. They suggested that – the cubic unit cells used for the simulation of the mechanical behavior can be understood as small representative volume elements taken at random from the larger cell.

Table 2.5

Calculated strain hardening coefficient for different particle arrangements

Particle arrangement	Random	Regular	Clustered	Gradient (Y)	Gradient (Z)
N	0.1284	0.193	0.1676	0.1227	0.1543

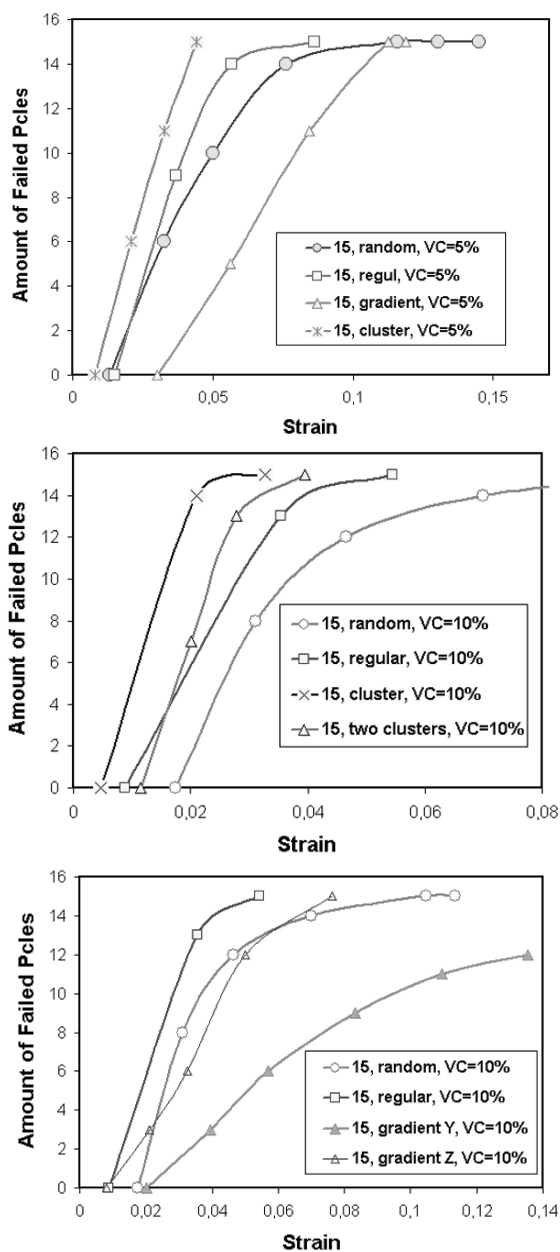


Fig 2.40 Amount of failed particles plotted versus the far field strain: (a) 15 particles, VC=5% , (b, c) 15 particles, VC=10%

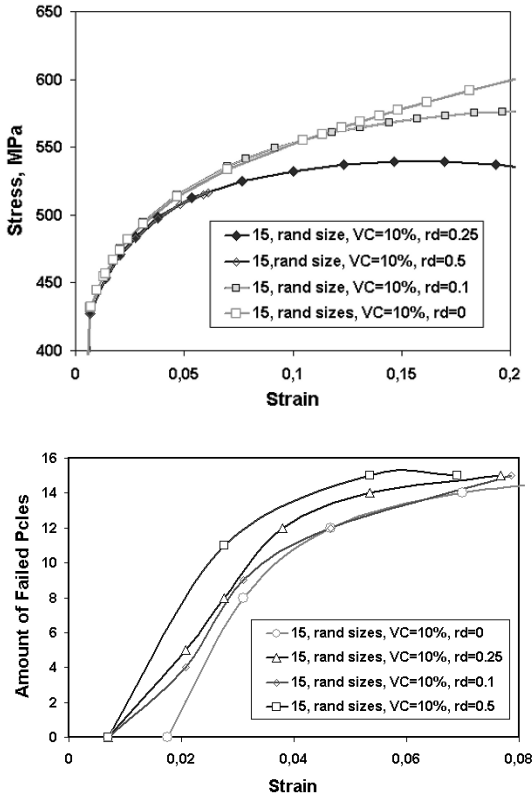


Fig 2.41 Examples of microstructures with particles of randomly distributed sizes (a), and stress-strain curves (b) and the amount of failed particles plotted versus the far-field strain (c) for these microstructures. $rd = \Delta r/r$

Table 2.6

Nearest-neighbor distance between particle centers the considered microstructures.

Microstructure	Average NND, mm	SEPD of NND	NNI
Random	12.69	2.55	1,17
Clustered	2.70	1.26	0.25
Gradient	5.85	2.31	0.54

Abbreviations: SEPD – statistical entropy of the probability distribution, NND- nearest-neighbor distance between particle centers, NNI- nearest neighbor index (ratio of observed nearest neighbor distance to the mean random distance)

Following this idea, we generated unit cells of the size 100x100x100 mm with random, clustered and uniform particle arrangements using the same algorithms as for the simulated cells. The values of NND, NNI and the entropy of NND, determined from the cells, are given in table 2.6. The scattering of the distribution of NND, characterized by the statistical entropy of the distribution, decreases with decreasing the average value of NND.

One can see that the generated random microstructures is really close to the ideal random ($NNI = 1.17$ versus 1.0 in the ideal case) and that the degree of clustering in the generated gradient and clustered microstructures is rather high.

From the simulations presented in this paragraph, one may draw the following conclusions. The arrangement of particles influences first of all the strain hardening rate, and the damage behavior of composites. This is a remarkable difference from the effect of the volume content of inclusions, which influences the flow stress, not just its slope, i.e., strain hardening rate.

The regular particle arrangement ensures highest flow stress of a composite, especially, after the particle failure begins. The discrepancy between our results and results by Segurado et al. [7] in this point is discussed above. The clustered particle arrangement leads to a very high damage growth rate, and to a low critical applied strain. However, no negative effect of particle clustering on the effective response of the composite was noted. This conclusion is in agreement with the numerical conclusions by Segurado et al. [7] (“the increase in strength due to clustering is almost negligible for the matrix and reinforcement properties typically found in metal matrix composites”).

Effect of the variations of particle sizes on the damage evolution

At this stage of the work, the effects of scattering of particle sizes and local strength on the effective response and damage behavior of the composite were investigated.

In order to vary the particle sizes, microstructures with randomly arranged particles of random sizes were generated. The radii of particles were assumed to follow the normal probability distribution law. The degree of scattering of particle sizes, which was characterized by a standard deviation of the normal distribution law, was varied at the level of 0.1, 0.25 and 0.5 of the average particle radius (which was 1.1676 mm, for the cell with 15 particles and 10% of volume content). In order to keep the volume content of particles constant, the randomly distributed radii of particles were normalized. Table 2.7 gives the maximum and minimum sizes of particles for the considered values of the standard deviations. Fig. 2.53(a) shows the arrangements of the particles for different deviations of the probability distribution of the particle sizes. Fig. 2.53(b) and (c) shows the tensile stress-strain curves (b) and the amount of failed particles (c) plotted versus the far-field strain, for these microstructures.

One can see from Fig. 2.53(a) that the variations of the particle sizes cause a strong decrease in the strain hardening rate of the composite during the elastoplastic deformation with damage. The differences in the effective responses of the composites with different scattering of particle sizes are negligible in the elastic region, but become rather large when the particles begin to fail, and increase with increasing the density of failed particles. From Fig. 2.53(b) it can be seen that the damage evolution in the particles begins at some lower applied strain when the particle sizes vary (0.069 versus 0.175 mm, when the particle radii are constant). Also, the critical applied strain is about 22% lower for the random particle sizes with the standard deviation 0.5 r , and about 60% lower for the random particle

sizes with the standard deviation $0.25r$, than for the homogeneous particle radii. The difference between the cases of the constant particle radii and the randomly distributed with the deviation $0.1r$ is negligible, but becomes rather large for the deviations of 0.25 and $0.5r$. Therefore, the scattering of particle sizes leads generally to the quicker and earlier damage growth in the composites.

Table 2.7

Maximum and minimum sizes for considered probability distributions of the particle radii

Standard deviation of radii/mean radius	Value of the standard deviation of r	Maximum particle radius	Minimum particle radius
$\Delta r/r$	Δr	$r_{\max}$	$r_{\min}$
0.10	0.1168	1.6595	0.7021
0.25	0.2919	1.8506	0.6282
0.50	0.5838	1.9951	0.1582

Discussion

Fig. 2.41(a) shows the values of the flow stresses, corresponding to the applied displacement $u = 0.15$ mm, for all the unit cells with 15 particles and volume content 10% as a column charts. For comparison purposes, the values of flow stresses for the regular particle arrangements with volume contents 5% and 15% are shown.

The column charts of the critical applied strain, shown in Fig. 2.41(b), illustrates the effect of the particle arrangement on the damage growth in the composites. Comparing Fig. 2.41(a) and (b), one may see the general tendency: the higher is the stiffness and the flow stress of a composite, the lower critical failure strain should be expected. (There are however some deviations from this relation.). Fig. 2.43 shows the critical applied strain (at which the linear “quick growth” part of the curve of the fraction of failed particles versus far-field strain goes into “asymptotic” part of these curves) plotted versus the flow stress of the composite at the displacement 0.15 mm for all the cells with 15 particles. From table 2.6 and Fig. 2.41, one can see that there is no monotonic relation between parameters of particle clustering and the effective response or rate of particle failure in the composites.

Considering the ranking of the microstructures in Fig. 2.41 one can see that the gradient microstructures demonstrate a very high damage resistance as compared with the isotropic (random, uniform and clustered) microstructures. The isotropic (random, uniform or clustered) microstructures are grouped in the left part (low critical strain) of the figure. From all the isotropic microstructures, the clustered microstructure ensures the lowest damage resistance.

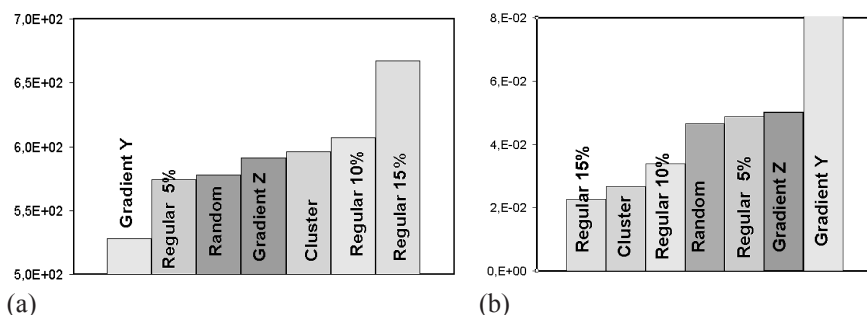


Fig 2.42 Flow stress (at the displacement load $u = 0.15$) (a) and critical far-field applied strain (b) for different particle arrangements. VC = 10% (if not marked)

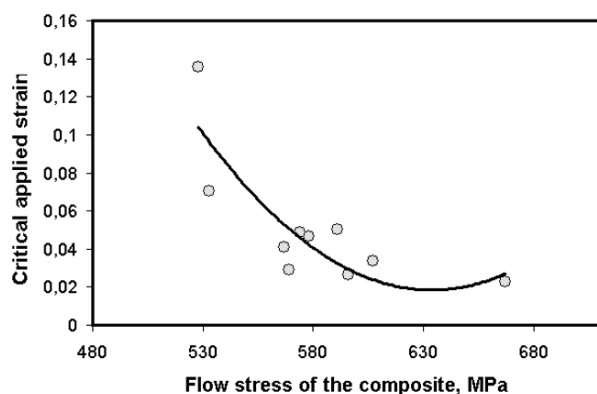


Fig. 2.43 Critical applied strain plotted versus the flow stress of the composite (at the far-field strain 0.15 mm) for all the cells with 15 particles and VC = 10%.

In this relation, the big different between the mechanical behavior of the gradient Y (gradient particle arrangement with a gradient vector coinciding with the loading vector) and gradient Z (gradient particle arrangement with a gradient vector normal to the loading vector) composites is of interest. Both microstructures (gradient Z and gradient Y) show high damage resistances, but the flow stress of these structures differs. The effect of the orientation of the gradient vector on the flow stress and damage resistance of the composite can be explained by using an (over-simplified) illustrative representation of the gradient material as a bilayer material, consisting of a plastic layer (i.e., the part of the composite with a low content of particles) and a stiff layer (i.e., the part of composite with a very high content of particles). If the material is loaded along to the gradient direction, the stiffness of the material is controlled by the stiffness of the high particle density region (which is rather firm, and, on the other hand, allows quick failure of many particles due to the high local deformation, according to the results of paragraph 3.3). Therefore, the stiffness of the gradient Z composite is quite high, and the particle failure goes rather quickly. In the case of gradient Y, the plastic flow of the material is controlled by the lower sections of the specimen with the small density

of particles. Therefore, the flow stress of such a material is quite low (close to the flow stress of the pure matrix). The region of high particle density does not form a load bearing construction, and is therefore not subject to a quick failure of particles. One can draw a conclusion that if the regions of high particle density are arranged in such a way that they form a bearing construction (gradient Z structure) or play a role of a “super-reinforcement” (clustered structure), that leads to a quick failure of many particles in the regions. Otherwise, if the high particle density regions does not form a load-bearing construction (gradient Y microstructure), the flow stress of the material is relatively low (since the plastic flow is controlled by the regions of low particle density), yet, the intensity of damage failure is relatively low as well.

Conclusions

Numerical analysis of the effect of microstructure, arrangement and volume content of hard damageable inclusions in plastic matrix on the deformation and damage growth has been carried out. On the basis of the numerical testing of different microstructures, the following conclusions have been drawn.

The stiffness and flow stress of the composites can be controlled both by the volume content of the hard particles, by the degree of localization (clustering) of their arrangement, and by shape and orientation of the regions of high particle density.

Flow stress of composite increases with increasing the volume content of particles. An increase in the volume content by 5% leads to the increase of the flow stress by approximately 4%. The amount of particles (at the same volume content) influences the effective response of the material only at rather high stage of particle failure, when many particles failed already. In this case, the flow stress is higher for a composite with a higher amount of particles. The higher the volume content of particles, the lower is the far-field applied strain, at which the most of the particles fail. An increase of the volume content of particles by 5% leads to the decrease of the load at which the total failure of particles is observed by 4...5%.

The particle arrangement does not influence the effective response of the material in elastic area or at small plastic deformation. The effect of the particle arrangement on the effective response of the material becomes significant only at the load at which the particles begin to fail. After the first particle fail, the flow stress of the composite and the strain hardening coefficient increase with varying the particle arrangement in the following order: gradient < random < clustered < regular microstructure. The applied strain, at which the most particles fail, decreases in the following order: gradient > random > regular > clustered.

The variations of the particle sizes causes very strong decrease in the strain hardening rate and leads to the quicker and earlier damage growth in the composites. The differences in the effective responses of the composites with different degree of scattering of particle sizes are negligible in the elastic region, but become rather large when the particles begin to fail, and the differences increases with increasing the density of failed particles.

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2.3.2 Step-by-step packing approach to the 3D microstructural model generation and quasi-static analysis of elasto-plastic behavior of composites⁶

In the last few decades great progress has been made in mechanics and physics of solids, which provides new knowledge of material behavior under loading and substantially promotes our understanding of physical mechanisms of deformation and fracture. Over the recent years a new scientific trend – physical mesomechanics has been developed on the basis of a concept of multiscale nature of deformation and fracture processes. In the frame of mesomechanical methodology [14, 15, 17, 19, 28], a solid under loading is considered as a complex system of structural levels – micro, meso and macro, with deformation going on different scale levels in a self-consistent way. For instance, individual dislocations observed at the initial stage of loading tend to organize into cellular and band structures which, in turn, go on to form mesoscale shear bands. Plastic strain localization at the mesoscale level precedes macroscopic neck formation and fracture of the specimen.

A great body of experimental and theoretical data, e.g. [4, 11, 13-15, 17-19, 28, 29, 33], indicates that stress and strain distributions on the mesoscale are characterized by essential non-homogeneity attributed to the structural effects. Although an average response of a representative mesovolume assumes to agree with the experimental stress-strain curve which represents the macroscopic behavior of the material, local values of stresses and strains on the mesoscale can deviate widely from the average values [4, 11, 13-15, 19, 28, 29]. It is, therefore, a challenge to estimate stress-strain fields on the mesoscale level. In the context of this task a numerical simulation shows good promise as a research tool in addition to experimental methods.

A series of computational works [22, 24-27] has been devoted to the numerical simulation of deformation and fracture processes in heterogeneous materials with explicit consideration of their three-dimensional microstructure. In order to introduce in calculations a 3D-structure a method of a step-by-step packing (SSP) to design artificial three-dimensional structures similar to real ones by geometrical and statistical characteristics of their constituents has been developed in [22, 26].

The method proposed has been applied in [22, 24-27] to calculations of several test examples of polycrystalline and composite structures without providing a comprehensive analysis of their stress-strain behavior. First test calculations have been performed in [22, 25-27] for polycrystalline aluminum structures subjected to tension [22, 25] and shock wave loading [26, 27], using the finite-difference (FD) method [35].

In [25] the SSP-method has been applied to design a 3D MMC-structure consisting of Al(6061)-matrix and 10% of Al₂O₃-inclusions in a 50×50×50 cubic grid,

⁶ Reprinted from V.A. Romanova, E. Soppa, S. Schmauder, R.R. Balokhonov, “Mesomechanical analysis of the Elasto-Plastic behavior of a 3D composite-structure under tension”, *Comput. Mech.* 36, pp. 475-483 (2005) with kind permission from Springer

with using a procedure of excluding extra phases to obtain inclusions of uneven shape. FDM-calculations have been performed for the MMC-structure subjected to a complex quasistatic loading so that tensile displacements were given along X-direction, with two of the cube lateral faces being free of external forces and the rest three faces treated as symmetry planes. Influence of the composite structure and loading conditions on distributions of equivalent stresses and equivalent plastic strains on the surface and in the volume has been studied at specimen elongation of 0.24%. A comparative analysis of equivalent plastic strain distributions in the 3D MMC-structure and corresponding 2D-structures calculated in terms of plane strain conditions has been done in [24, 25]

The present work has its goal to examine in detail the stress-strain behavior of a MMC-structure subjected to quasistatic tension. In the frame of this contribution, the following tasks not addressed before in [22, 24-27] have been solved:

1. The SSP-procedure applied in [25] to design a two-phase structure consisting of Al(6061)-matrix and Al_2O_3 -inclusions is further modified to obtain inclusions more similar to real those in their geometrical and statistical characteristics. The computer-aided design of the MMC-structure is briefly considered in Section 2. Material constants and model parameters used in calculations as well as schematics of load application are given in Section 3.
2. The mechanical problem how far the dynamic formulation can be used for the description of quasistatic problems has been solved, using both the finite element (FE) [7] and finite-difference (FD) [35, 36] methods. Special attention has been given to the comparison of FE- and FD-calculations in order to test the explicit code applicability in solving the quasistatic problem.
3. Evolution of equivalent plastic strain during tensile loading has been investigated with a comparison of meso- and macro-scale processes.
4. The analysis of stress and strain distribution in the bulk of the specimen has been provided on the base of the mesomechanical concept, with special attention paid to the quantitative estimation of local characteristics on the mesoscale level. Particular emphasis has been paid on the investigation of individual contributions from different components of the stress and strain tensors to local and global response of the material.

Discussion of the computational results is presented below.

Microstructure set-up

The incorporation of a material structure, i.e. the distribution of different material properties throughout the volume, is a non-trivial problem in the case of three dimensional simulations. An even more complicated task is to introduce explicitly a *real* 3D-structure since it requires the information about structural patterns not only on the surface but also in the bulk of the specimen. Experimental techniques [3, 9] which could provide layer-by-layer structural images are, as a rule, rather

expensive and laborious. In the context of aforesaid, computer-aided modeling is considered to be a reasonable tool to design artificial 3D-structures similar to real ones by characteristics of their structural components, i.e. shape, size, volume content, spatial distribution etc.

In the general case, the design of a 3D-structure is reduced to the problem of packing a finite volume with structure elements without gaps and overlapping. Over the recent years, several methods of computer-aided simulation of microscopic heterogeneities have been developed, including Potts Monte Carlo Method [1], Voronoi tessellation [6], cellular automata [20], pseudo-front tracking method [8] and the phase-field approach [10] etc.. Some of them use a geometrical procedure to generate regular or irregular structures and others are based on certain physical principles and thermo-dynamic formulations. All of these were originally applied in two dimensional simulations and their main goal was to obtain reasonable conclusions regarding the kinetic and statistical aspects of a 2D grain growth. Although in recent works [21] some of these methods were successfully applied in a 3D case, realization of these techniques in three dimensions is for the most part a complicated task calling for optimization of computational algorithms since the memory and processing time requirements needed to make calculations increase dramatically with the increase of spatial dimensions.

In this paper, in order to design the composite structure whose mechanical behaviour will be further numerically investigated, use was made of a step-by-step packing (SSP) algorithm we proposed in [22, 26]. In contrast to the methods listed above [1, 6, 8, 10, 20, 21], this technique disregards physical and thermodynamical aspects of the microstructure evolution such as grain growth, phase coalescence, recrystallization and so on. Its goal is only to design a material structure similar to a real one, whose mechanical behaviour will be further numerically investigated.

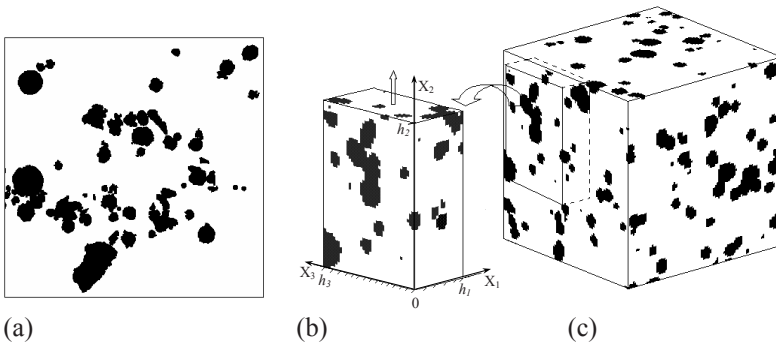


Fig. 2.44 (a) Binary image of the experimentally determined MMC-microstructure obtained by Dr. G. Fischer/ Universität Dortmund, Germany. (b) Schematics of load application to the MMC test-volume cut out from the SSP-designed composite structure (c).

The SSP-algorithm includes the following steps:

1. The volume to be packed with the structure is discretized with the computational grid and three-dimensional coordinates are defined for each discrete point. Since the design of a 3D-structure precedes the task of

simulating its mechanical behaviour, the test-volume geometry is defined from the conditions of an appropriate mechanical problem and the discretization parameters are dictated by the numerical method to be further applied.

2. Each discrete point of the volume is assigned a so-called structural index (SI) corresponding to a certain phase. Initial conditions imply that all points possess the same SI with the exception of those treated as nuclei of new phases.
3. The discrete volume is filled with structural elements in a step-by-step fashion. At each step in the processing time, the volumes surrounding the nuclei are incremented by preset values in accordance with given law of their growth. Such a procedure repeats until the volume fraction of the growing structural elements has reached the preset magnitude. The initial distribution of nuclei, the law of volume increments and the growth rate can be defined from the analysis of experimental data.

In this work the SSP-technique has been applied to design a MMC-structure composed of Al(6061)-matrix and vol.10% Al_2O_3 -inclusions, with the microstructure parameters of a real composite material [30-32]. The experimental data [30-32] indicate that Al_2O_3 -particles whose size is varied from 5 to 50 μm are characterized by rather irregular shape, fig. 2.44(a). It has been found that an appropriate microstructure model can be provided via the design of a two-phase composition with the predominant growth of one of its constituents. Initially the nuclei of two sorts were randomly distributed throughout the volume discretized preliminary by a cubic grid of $100 \times 100 \times 100$ elements, with the nuclei of both sorts in the ratio of 1:3. Although both phases developed simultaneously in accordance with the spherical law of homogeneous growth in all three spatial directions [26], the first one grew three times faster than the second one. The second phase which will be further treated as Al_2O_3 - particles stops to grow as soon as its volume content reaches the preset value of 10%, after that all unfilled places of the volume are assumed to be matrix in addition to those already possessing the matrix SI. The resulting structure contains 10% of inclusions of different sizes and shapes, fig.2.44(c).

Material properties and loading conditions

Apparently, the finer the computational grid, the better the agreement between statistical characteristics of the experimental and designed structures, provided that the SSP-laws applied in the simulation are correctly defined. This is the reason to design at first a reference structure in a sufficiently detailed computational grid of $100 \times 100 \times 100$, fig. 2.44(c). Note, however, the numerical solution of the three-dimensional mechanical problem places more stringent requirements upon the computer memory and processing time in comparison to those needed for the structure design. In addition, the memory requirements are several times higher when using the implicit solver [7]. Since this paper has its goal to compare numerical solutions obtained by implicit [7] and explicit [35] methods, size of the

test-structure has been chosen so as to satisfy the memory requirements imposed by the implicit code [7]. In this connection, further calculations have been performed for a smaller test-volume of $55 \times 41 \times 22$ elements, as a cut out from the reference structure as presented schematically in fig. 2.44(b-c). From the macroscopic point of view this test-volume is not representative since it contains only several inclusions whose total volume is about vol. 23%, with particle content in different planes varying from vol. 10 to 30 %. The reason for which this structure was chosen to be investigated is a sufficient amount of computational elements contained in the inclusions, which is important in view of the outlined goals to study non-uniform stress-strain patterns resulting from the structural heterogeneities.

Three-dimensional calculations of the MMC-structure behavior under quasi-static tension have been carried out, using both the finite-element (FE) [7] and the finite-difference (FD) [35, 36] methods. Referring to the schematics of loading, fig. 2.44(b), tension is applied to the surface $x_2 = h_2$ in the positive direction of the X_2 -axis, while the planes $x_1 = 0$, $x_1 = h_2$, $x_3 = 0$ and $x_3 = h_3$ are treated as free surfaces, and the movement of the plane $x_2 = 0$ is fixed parallel to the X_2 -axis. The lengths of the test-volume along the X_1 -, X_2 - and X_3 -axes are 22, 55 and 41 microns, respectively.

Table 2.8

Material constants and model parameters used in the calculations.

Property	Al(6061)-matrix	Al ₂ O ₃ -particles
Density, g/cm ³	2.7	3.99
Shear modulus, GPa	27.7	156.0
Bulk modulus, GPa	72.8	226.0
Young modulus, GPa	68.3	380.0
σ_0 , MPa	105.0	-
$\sigma_{\max}$, MPa	170.0	-
ε_0	0.048	-

According to the experimental data [30-32], Al₂O₃-particles under loading possess elastic behaviour, whereas the matrix undergoes elasto-plastic deformation. Since at the elongation of 0.5% crack nucleation and development have not been registered in the experiments except of already existing cracks and voids after extrusion [30], fracture processes were disregarded from consideration. In order to describe the strain hardening in the matrix we used the fitting function of Voce type as proposed in [32]:

$$\sigma_{eq} = \sigma_0 + (\sigma_{\max} - \sigma_0) \left(1 - \exp \left(- \frac{\varepsilon_{eq}^p}{\varepsilon_0} \right) \right) \quad (2.16)$$

Here σ_{eq} and ϵ_{eq} are the equivalent stress and the equivalent plastic strain, σ_{max} is the saturation stress, σ_0 and ϵ_0 are the equivalent stress and strain corresponding to the beginning of plastic yielding. Mechanical properties of matrix and inclusions as well as fitting constants are given in table 2.8.

Mesomechanical analysis and discussion of computational results

On application of explicit code in solving quasi-static problems

Although recent advances in computer technologies extend considerably the range of mechanical and physical problems feasible to be solved, the memory and processing time requirements remain to be a significant limiting factor in the case of three-dimensional calculations. Thus, the optimization of computational methods and numerical codes as well as simplification of mathematical models continue to be topical tasks in modern computational mechanics and materials science. These problems become even more acute for models explicitly incorporating the internal structure since it requires high resolution of computational grid for the structure elements to be described with an appropriate number of details.

From the viewpoint of memory requirements, explicit numerical codes are more efficient in comparison with implicit ones. Their use, however, is strongly limited by a stability condition which imposes a restriction on the time step to be less than that needed for the elastic wave to traverse one spatial interval of the computational grid. This almost unfailingly leads to a considerable increase in computational time when calculating quasi-static problems.

In spite of this disadvantage, explicit codes have been successfully used to solve quasistatic problems for both homogeneous and heterogeneous materials [4, 11-14, 23, 36, 37]. In [37] an explicit finite-difference method earlier developed in [34] for calculations of wave propagation in elasto-plastic media was applied in 2D- and 3D-simulations of a homogeneous aluminium plate under tension. Later in a series of computational works [4, 11-14, 23] this method was adapted to problems of heterogeneous materials with explicit consideration of their microstructure and applied in 2D-calculations of elasto-plastic deformation and fracture under quasi-static loading. It has been shown for materials non-sensitive to strain rate effects [4, 11, 23] that results of dynamic and static models well agree, provided that the loading rate is slowly incremented to minimize wave phenomena.

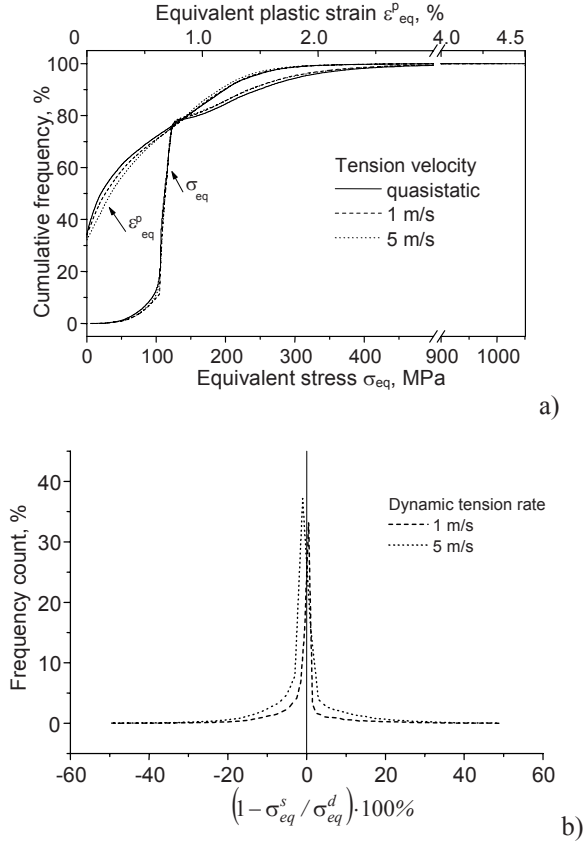


Fig. 2.45 Comparison of quasistatic(FEM) and dynamic (FD) calculations (true effective strain is 0.5%): a) cumulative frequency curves of equivalent stresses and plastic strains; b) normalized frequency count of deviation of quasistatic (σ_{eq}^s) and dynamic (σ_{eq}^d) equivalent stress fields. Note, the FD and FE methods give almost exact the same results.

The test-volume, fig. 2.44(b), was loaded by applying tension velocity to one of its ends with the other being fixed along the tensile axis. In order to reduce wave effects attributed to the dynamic model itself, the tension rate was smoothly incremented up to its constant value for the waves initiated at the loaded surface to traverse the test-volume length several times at each step of loading.

Presented in fig. 2.45 are the cumulative frequencies of equivalent stresses and plastic strains obtained in FEM- and FDM-calculations and the frequency count of difference between static and dynamic stress fields. The results demonstrate reasonable agreement at a tension rate of 1 m/s – the difference in dynamic and static stress-strain distributions is less than 10 % for most parts of the test-volume. Regarding the discrepancy of 20÷50% observed in several local regions ($\approx$ vol.

0.7%), the comparison of dynamic response at higher and lower tension rates leads us to the assumption that it is not associated with the strain rate effects but rather attributed to numerical codes themselves since both dynamic fields exhibit the same deviation from the static one. Presumably, the reason of this disagreement is a reduction of the dynamic solution accuracy in the areas of high stress-strain gradients. In order to avoid hour-glass distortions of the computational grid in the implicit calculations use was made of an artificial viscosity [36] which can become considerable in the areas of high stress-strain gradients, reducing the accuracy. This conclusion has been additionally confirmed by a layer-by-layer analysis of dynamic and static stress-strain patterns, which has shown that the higher the stress-strain gradients in local areas, the more the disagreement between static and dynamic results. Conceivably, this disagreement can be minimised by smoothing of structure interfaces or mesh refinement.

At a loading rate of 5 m/s in the FD-simulation the deviation of dynamic and static stress-strain fields increases due to the strain hardening in matrix – the higher the loading rate, the weaker the plastic strain localisation effects. Such a disagreement should be taken into account when estimating material quasistatic response, based on the results of dynamic calculations.

In the light of aforesaid, we come to the conclusion that the dynamic code is applicable to simulations of a quasistatic response of the MMC-structure within the range of loading rates below 1 m/s, provided that the rate of loading smoothly increases up to its constant value. The use of the explicit code is expected to allow one to make 3D-calculations for a representative MMC-structure with a high resolution of the computational grid, with essentially reduced computer memory requirements.

It should be noted, however, that this conclusion cannot be extended to the case of other materials and loading conditions without additional calculations. Each kind of structure and method of loading calls for special tests in order to determine the range of strain rates in which dynamic effects become insignificant in regard to the stress-strain behaviour at the meso- and macro-scale levels.

Analysis of plastic strain evolution

In the 3D case, along with the complexity of the numerical solution, visualisation and analysis of the results also become more difficult. Due to its heterogeneity, every layer of the test-volume exhibits an individual stress-strain pattern that, in addition, evolves in time. In this paper we, therefore, give only some representative illustrations of plastic strain patterns in planes selected, with the conclusions drawn for the general case.

A step-by-step and layer-by-layer analysis of the plastic strain distribution has shown that first plastic shears take place on the test-volume surface. It is well-known [14-17, 19, 28] that geometrical special features of the specimen itself, such as corner points, notches, free surfaces and so on, result in strong stress concentration on the macroscopic level. In [22] we have shown for the case of a 3D polycrystalline material that the equivalent stress on the surface is higher than that in the bulk of the specimen.

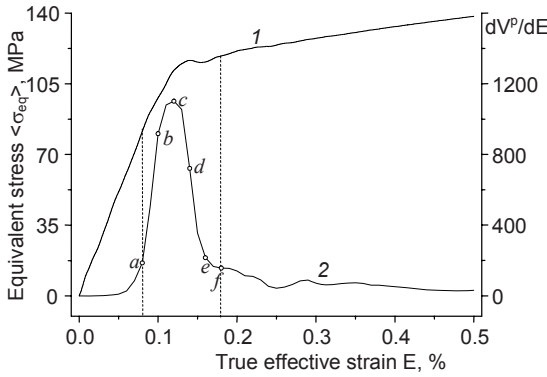


Fig. 2.46 Average equivalent stress (curve 1) and derivative of matrix volume V^P involved into plastic deformation (curve 2) vs. true effective strain.

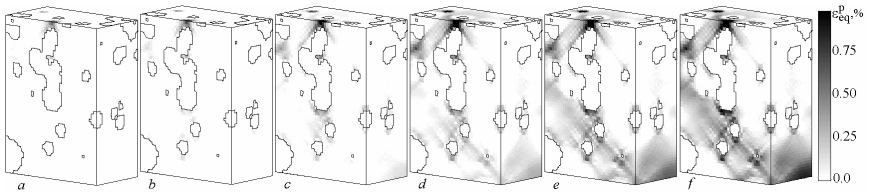


Fig. 2.47 Plastic strain patterns on the surface at different elongations of the test-volume (refer to fig. 2.46).

The reason is that normal components of the stress tensor on the surface are known to be zero, whereas in the volume all stresses make their contribution to the equivalent stress, reducing its value.

This conclusion, however, cannot be extended to the general case of composite materials. Due to considerable differences in elastic properties of matrix and inclusions, incompatible deformation and, as a result, stress concentrations in the vicinity of interfaces can result in higher stress concentrations in some internal regions than that caused by the surface effects, which can lead to crack origination not on the surface but in the bulk of the material [2]. This situation becomes even more unpredictable in the case of inclusions of an irregular shape. This was the reason, therefore, to check whether this conclusion holds for the MMC-structure under study.

Plotted in fig. 2.46 are the average equivalent stress and the increment of the matrix volume plastically deformed vs. true effective strain of the specimen. Here

and below the equivalent stress σ_{eq} and its average value $\langle \sigma_{eq} \rangle$ are calculated as follows:

$$\sigma_{eq} = \sqrt{\frac{3}{2} \sigma_{ij} \sigma_{ij}} \quad (2.17)$$

$$\langle \sigma_{eq} \rangle = \frac{1}{V} \int_V \sigma_{eq} dV \quad (2.18)$$

where σ_{ij} are the stress tensor components, σ_{eq} is the equivalent stress, and V is the computational volume, with the i - and j -indices varied within the range of 1 to 3. Note, in the general case of a 3D heterogeneous material the average equivalent stress calculated by eq. (2.18) can deviate from both true and nominal stresses as obtained in experiments and cannot be directly associated with the experimental stress-strain curve without additional verification.

Refer to fig. 2.46, due to couple effects of tensile loading and strain hardening, plastic strain accumulation in the places already involved into yielding and origination of new plastic shears in elastically-deformed areas go alternately. Stress concentration in the vicinity of interfaces takes place from the very beginning of loading, which gives rise to plastic shear nucleation in local areas of matrix material at true effective strain of 0.004% which is ≈ 2.7 times less than the preset value of the yield strain ε_0 (see table 2.8). This phenomenon qualitatively agrees with the experimental findings in the field of microplasticity e.g.[5].

From the appearance of the first plastic shears and up to the true effective strain of 0.12% the matrix volume undergoing plastic deformation rapidly increases, which indicates a primary role of the nucleation of new plastic shears in this region. After the plastically deformed volume reaches $\approx 33\%$ of the matrix, the rate of shear nucleation in new regions drastically decreases, that corresponds to the beginning of the strain hardening part in the average stress – true effective strain curve. The evolution of plastic strain patterns on the surface at this stage of loading is illustrated in fig. 2.47.

After plastic deformation covers $\approx 63\%$ of the matrix, the curve 2 flattens out, which indicates that new regions are no longer involved into plastic yielding but plastic deformation continues to develop in the shear bands already formed. Summarizing, the formation of plastic strain localization areas is mostly completed at the stage associated with the linear part of the average stress – true effective strain curve, whereas intensive development of plastic deformation in the already formed shear bands corresponds to the stage of macroscopic strain hardening.

Stress and strain distributions on the mesoscale level

Plastic strain patterns in different planes of the 3D test-volume are mainly controlled by both microstructure distribution and orientation of the plane relative to the axis of tension. Let us consider plastic strain localization in specimen cross-sections located parallel (fig. 2.48) and perpendicular (fig. 2.49) to the axis of elongation.

From the macroscopic point of view, the parallel- and perpendicular-oriented planes are in different conditions of loading. In the first case, fig. 2.48, planes $x_1 = \text{const}$ undergo tension along the x_2 -axis and compression along x_3 , which results in the formation of a system of shear bands in the matrix material.

First, plastic shears nucleate near interfaces in the regions of high stress concentration which is attributed to both incompatible deformation in the places of matrix and inclusion contact and uneven contours of the interfaces. Orientation of the shear bands at an angle of $\approx 45^\circ$ to the axis of elongation is primarily dictated by the loading conditions.

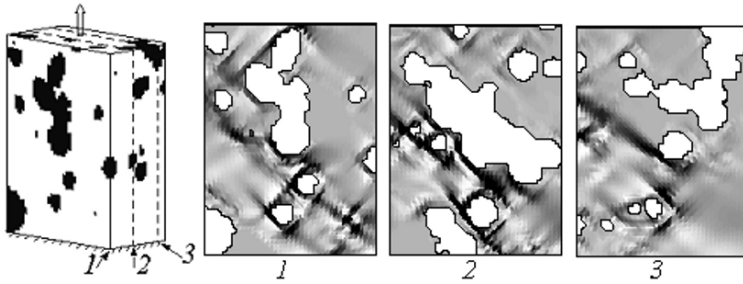


Fig. 2.48 Shaded relief maps of equivalent plastic strains in the selected planes parallel to the axis of tension. True effective strain is 0.5%.

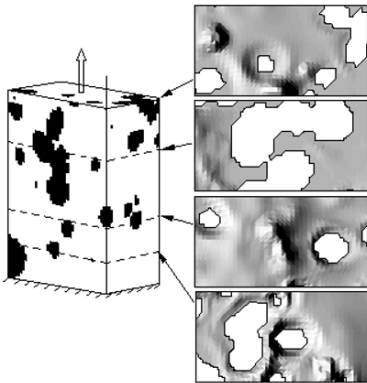


Fig. 2.49 Shaded relief maps of equivalent plastic strains in planes selected perpendicular to the axis of tension. True effective strain is 0.5%.

In planes $x_2 = \text{const}$ placed perpendicular to the axis of tension, fig. 2.49, the material undergoes two-axial compression, which prevents shear band formation but gives rise to the plastic strain localisation around inclusions, becoming especially pronounced in the vicinity of their boundaries.

Let us analyse in more details a contribution from different components of stress and plastic strain tensors to the stress and strain patterns. Presented in fig. 2.50 are the frequency count curves of stress and strain tensor components at a true effective strain of 0.5%. The frequency distribution of stress tensor components, fig. 2.50(a), calculated with steps of 5 MPa, was normalized as $(q_i/N_c) 100\%$, where q_i is the number of computational elements within the i -th interval, and N_c is the total number of grid cells. Excepting σ_{22} which represents the material response in the direction of tension, all components of the stress tensor demonstrate a symmetric distribution, with the axis of symmetry along $\sigma_{ij} = 0$ and the frequency peaks on this line. Since the matrix takes up 67% of the total volume, it is reasonable to suggest that the stress value corresponding to the highest frequency correlates to a greater extent with the average stress in matrix.

In order to describe the plastic behaviour we used the von Mises yield criterion [7, 34, 37], according to which the material response to loading becomes plastic, provided that the second invariant σ_{eq} of the stress tensor reaches its critical value. It is interesting, therefore, to analyse the contribution of different stress components to the value of equivalent stresses calculated by Eqn. (2.17). From the analysis of the curves plotted in fig. 2.50(a), σ_{22} gives the most significant contribution to the magnitude of σ_{eq} , with the frequency peak corresponding to ≈ 107 MPa. Note, the stress value is $\approx 23\%$ lower than that representing the average material response (point a in fig. 2.46).

The difference in these values well correlates with the volume content of Al_2O_3 -particles, which suggests that the maximum frequency corresponds to the stress field in the matrix, whereas the average equivalent stresses are mostly determined by the stress fields in particles. In addition, a contribution from the other stress components to the material average response also appears to be considerable. Even though their values in matrix are close to zero, they demonstrate high stress concentration inside the inclusions and especially in the vicinity of interfaces.

Frequency curves for components of the plastic strain tensor in the matrix, calculated with steps of 0.01%, are plotted in fig. 2.50(b). These curves demonstrate the presence of places undergoing tension, compression, shear and their combination as well. Refer to the extreme and average stress and strain magnitudes given in table 2.9, all components of stress and plastic strain tensors vary in a wide range including positive and negative values. Taking into account that the negative diagonal components correspond to tension and positive ones describe compression along appropriate directions, it is interesting to mark that even σ_{22} and ε_{22}^p take negative values in several local points, which means that these areas are under compression in spite of the external tension applied in the same direction.

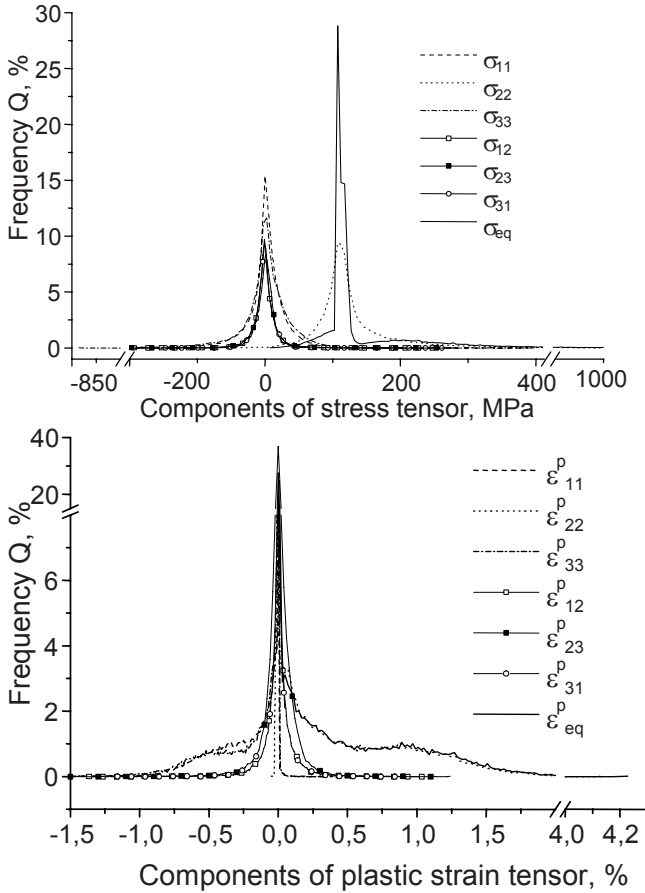


Fig. 2.50 Frequency count of stress tensor components (a) and plastic strain tensor components (b), obtained in FD-calculations (true effective strain is 0.5%).

This is a prominent illustration of specific effects attributed to a three-dimensional heterogeneity. One of the discussed topics of computational mechanics is whether two-dimensional continuum models are capable to provide a reasonable description when modelling deformation and fracture in heterogeneous materials with an explicit consideration of their microstructure and, if so, what are the frames of their applicability. Summarizing our previous experience in the field of 2D- and 3D calculations of heterogeneous media [22, 24-27], we come to the conclusion that each kind of structure and condition of loading requires special consideration to answer the question.

Although 2D-calculations are not presented in this paper, we can make some conclusions regarding this topic, based on the 3D-analysis of the stress and strain tensors. In both cases of plane strain and plane stress conditions the models are

reduced to a two-dimensional problem under the assumption that certain components of the stress and strain tensors are equal to zero all over the volume. In the case of the 3D MMC-structure subjected to tension as preset above, all components of stress and plastic strain tensors in the vicinity of interfaces and in the bands of localised deformation, respectively, deviate widely from zero and, thus, make their contribution to the local values of the stress and strain tensors (see table 2.9). Due to their small relative volume, the regions demonstrating the highest values of stresses and strains do not make a considerable contribution into the average material response. So in the case of macroscopic simulation, one- and two-dimensional models provide quite satisfactory results and the heterogeneous fields on the mesolevel can be ignored without serious consequences. It should be noted, however, that the correct estimation of local characteristics takes on great significance for materials whose deformation and fracture behaviour is strongly determined by mesoscale processes and then structural effects have to be taken into account.

Table 2.9

Average and extreme values of stress and plastic strain tensor components at true effective strain 0,5%.

ε_{ij}^p	$\langle \varepsilon_{ij}^p \rangle$, %	$\varepsilon_{ij \min}^p$, %	$\varepsilon_{ij \max}^p$, %	σ_{ij}	$\langle \sigma_{ij} \rangle$, MPa	$\sigma_{ij \min}$, MPa	$\sigma_{ij \max}$, MPa
ε_{11}^p	-0.234	-2.361	0.303	σ_{11}	-0.004	-695.1	387.0
ε_{22}^p	0.493	-0.058	4.131	σ_{22}	127.5	-324.1	1017.6
ε_{33}^p	-0.246	-2.476	0.396	σ_{33}	-0.01	-844.7	396.5
ε_{12}^p	-0.0007	-1.365	1.056	σ_{12}	-0.05	-193.5	265.9
ε_{31}^p	-0.0086	-1.161	0.873	σ_{31}	0.01	-147.1	283.1
ε_{23}^p	0.003	-1.763	1.238	σ_{23}	-0.06	-197.3	272.7
ε_{eq}^p	0.53	0.0	4.237	σ_{eq}	138.4	8.4	1017.3

Conclusions

Numerical investigation of the elasto-plastic behavior of a composite material under loading has been carried out, with taking into account its 3D structure. The analysis of stress and strain distribution in the bulk of the specimen has been provided in the frame of the mesomechanical concept, with special attention paid to the estimation of local characteristics on the mesoscale level. Deformation patterns in planes oriented parallel and perpendicular to the axis of tension have been studied. Particular emphasis has been paid on the estimation of individual contributions from different components of the stress and strain tensors to local and global response of the material. It has been shown that, due to its structural

heterogeneity, material on the mesoscale level exhibits a complex stress-strain behaviour, with the stresses and strains in local areas (e.g. in the vicinity of interfaces) deviating from their average level by several orders of magnitude.

To introduce in calculations the three-dimensional MMC-structure, use was made of a SSP-algorithm proposed in [22, 26]. The benefit of this method is, undoubtedly, its simple computer-aided realization with the minimal requirements of the memory and computational time. The disadvantage is that the application of an artificial structure makes impossible a direct comparison of computational and experimental results on the mesoscale level. However, this does not exclude the possibility of an indirect verification of this type of modelling. In the assumption that macroscopic responses of a real material and its artificial model should coincide when considering a representative volume, their comparison might be a proper test to verify computational results.

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