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Representative volume: Existence and size determination

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Abstract

The concept of the representative volume element (RVE) is analysed in the present paper. For elastic materials the RVE exists and one can determine the size of the RVE. However, for other applications, such as the case of softening materials, the RVE may not exist. In the present work the RVE has been investigated for different stages of the material response, including pre- and post-peak loading regimes. Results were based on a statistical analysis of numerical experiments, where tests have been performed on a random heterogeneous material.

Keywords: Representative volume element (RVE); Elasticity; Softening materials; Heterogeneous materials

1. Introduction

In certain applications where CPU time and memory are issues of concern, it is appealing to describe the structure with the help of a much smaller specimen, which is still large enough to be constitutively valid. This specimen, which is small enough on the one hand and large enough on the other, has been referred to as a representative volume element (RVE). Generally, in applications it is assumed that an RVE exists and that the size of it is initially prescribed. However, in our opinion the existence of an RVE for the class of quasi-brittle materials which show a strong softening response is one of the major questions to be answered. This issue has not been addressed sufficiently in literature, notable exceptions being [28,20].

Once the question of an RVE existence is positively answered, a procedure to find its size can be introduced. Several attempts have been made in literature to develop a procedure to determine the representative volume, see for instance [12,8,9,1]. An objective method to determine the size of the RVE was also proposed in [18,19]. This method is based on the combined statistical analysis of the numerically modelled material response. A more detailed description of this method will be presented below.

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However, in order to answer the question of existence and start developing the procedure to find a representative size, an RVE should be properly defined. Some definitions of an RVE, used by scientists for different purposes, are listed below

- The RVE is a sample that (a) is structurally entirely typical of the whole mixture on average, and (b) contains a sufficient number of inclusions for the apparent overall moduli to be effectively independent of the surface values of traction and displacement, as long as these values are *macroscopically uniform* [23].
- An RVE is the minimal material volume, which contains statistically enough mechanisms of deformation processes. The increasing of this volume should not lead to changes of evolution equations for field-values, describing these mechanisms [44].
- The RVE must be chosen *sufficiently large* compared to the microstructural size for the approach to be valid, and it is the smallest material volume element of the composite for which the usual spatially constant *overall modulus* macroscopic constitutive representation is a sufficiently accurate model to represent the mean constitutive response [12].
- The RVE is a model of the material to be used to determine the corresponding effective properties for the homogenised macroscopic model. The RVE should be large enough to contain sufficient information about the microstructure in order to be representative, however it should be much smaller than the macroscopic body (This is known as the Micro–Meso–Macro principle [22].).
- The RVE is defined as the minimum volume of laboratory scale specimen, such that the results obtained from this specimen can still be regarded as representative for a continuum [45].
- The size of the RVE should be large enough with respect to the individual grain size in order to define overall quantities such as stress and strain, but this size should also be small enough in order not to hide macroscopic heterogeneity [14].

All definitions reveal that the RVE should contain enough information on the microstructure yet be sufficiently smaller than the macroscopic structural dimensions. Thus, a separation of scales should be enabled. As [33] pointed out,

- The RVE is very clearly defined in two situations only: (i) unit cell in a periodic microstructure, and (ii) volume containing a very large (mathematically infinite) set of micro-scale elements (e.g. grains), possessing statistically homogeneous and ergodic properties. In other words in order to determine an RVE it is necessary to have (a) statistical homogeneity and ergodicity of the material; these two properties assure the RVE to be statistically representative of the macro response, and (b) some scale L of the material domain, sufficiently large relative to the micro-scale d (inclusion size) so as to ensure the independence of boundary conditions [33].

Periodic microstructures could be treated by continualisation or homogenisation methods. Traditionally, RVE sizes are defined as a minimum size of a microstructural cell that fulfils the requirement of statistical homogeneity. As such, it is a *lower bound*: larger microstructural cells behave similarly while smaller microstructural cells do not.

This paper is organised as follows: after discussing a test setup and some implementational issues in Section 2 the question of RVE existence is scrutinised – first, on the basis of a statistical analysis – Section 3, and then in connection with the size effect theory – Section 4. Section 5 deals with the RVE size determination: the literature overview on this question, given in the beginning of the Section, is followed by a novel method to determine the RVE size. Question of the importance of using the periodicity both material and of boundary conditions is addressed in Section 6. Finally, Section 7 concludes the paper.

2. Test set-up and implementational issues

A random heterogeneous material is introduced in this paper as a three phase material, specifically a material with matrix, inclusions (here, in a circular shape) and an interfacial transition zone (ITZ) surrounding each inclusion. Each material component has its own set of properties in terms of Young's modulus and Poisson's ratio. Here it is chosen that inclusions and ITZ have the highest and the lowest stiffness, respectively. Sizes of inclusions vary from [2.5 mm to 5 mm] (with a uniformly random distribution) and the thickness of the ITZ has been chosen as 0.25 mm, i.e. 10% of the smallest diameter of the inclusions. The material components properties are presented in Table 1 and used throughout this paper. The material with the above properties could be a representation of concrete, but generally, any three phase composite material could be described.

In order to address the question of RVE existence, a statistical analysis has been employed. First of all, a series of samples with increasing sizes are produced (Fig. 1), sizes vary from 10×10 mm^2 till 25×25 mm^2, and then for each sample size different inclusion locations (with a fixed value of volume fraction of inclusions) are constructed (Fig. 2). This procedure is repeated for several values ρ (30%, 45% and 60%) of volume fractions of inclusions (Fig. 3).

Table 1
Material components properties

	Inclusions	Matrix	ITZ
Young's modulus [MPa], E	30,000	25,000	20,000
Poisson's ratio [–], v	0.2	0.2	0.2

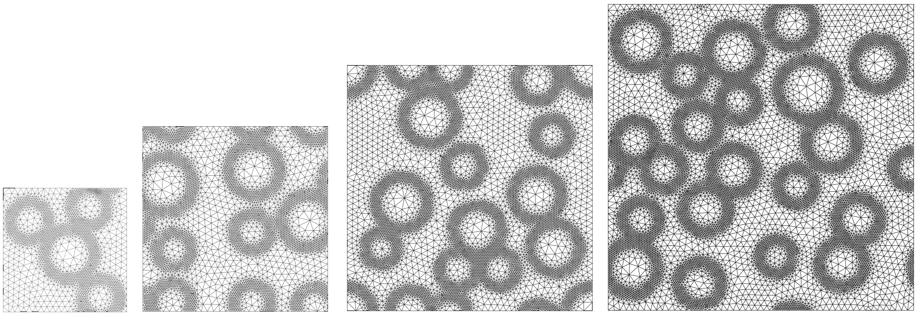

Fig. 1. Sizes of the sample, from left to right 10×10 mm^2; 15×15 mm^2; 20×20 mm^2; 25×25 mm^2 ($\rho = 30\%$).

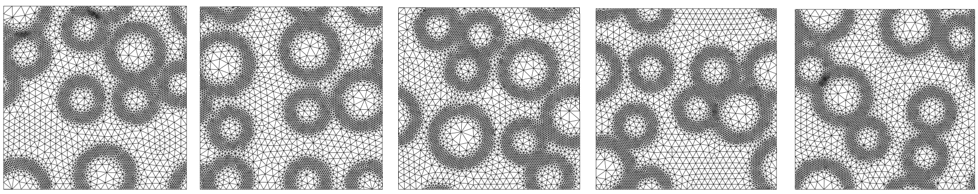

Fig. 2. Different realisations of the sample for size 15×15 mm^2, $\rho = 30\%$.

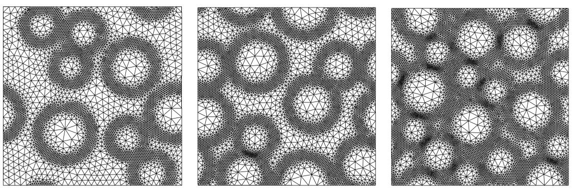

Fig. 3. Volume fractions of inclusions, from left to right $\rho = 30\%$; $\rho = 45\%$; $\rho = 60\%$ for size 15×15 mm^2.

2.1. Constitutive law

An elasticity-based gradient damage model [30,34,39] is used for the materials component description:

$$\sigma = (1 - \omega)D^e : \varepsilon \tag{1}$$

where σ and ε are stresses and strains, respectively, D^e is the matrix of elastic stiffness and ω is a damage parameter. The damage parameter ω is described as a function of the history-dependent parameter κ: $\omega = \omega(\kappa)$. The exponential softening law is employed here as an evolution law

$$\omega = \begin{cases} 0 & \text{if } \kappa < \kappa_0 \\ 1 - \frac{\kappa_0}{\kappa}(1 - \alpha + \alpha \exp(-\beta(\kappa - \kappa_0))) & \text{if } \kappa \geqslant \kappa_0 \end{cases} \tag{2}$$

Model parameters α and β represent the residual stress level and the slope of the softening curve, respectively. The crack initiation strains and length-scale parameters (here, for simplicity, chosen to be equal for all three phases) are specified in Table 2. Note, that the crack initiation strain of the inclusions has been chosen artificially high in order to avoid crack propagation through the inclusions. The material behaviour is regularised by means of gradient-enhancement, in particular, the implicit gradient damage model of Peerlings [34] is used, whereby a non-local equivalent strain is computed from a local equivalent strain according to

$$\bar{\varepsilon} - \frac{1}{2}\ell^2 \nabla^2 \bar{\varepsilon} = \tilde{\varepsilon} \tag{3}$$

where $\tilde{\varepsilon}$ is a local equivalent strain, $\bar{\varepsilon}$ is a non-local equivalent strain, ℓ is the internal length of the non-local continuum, related to the scale of the microstructure. Eq. (3) is accompanied by homogeneous natural boundary conditions, which imply continuity of the non-local equivalent strain across inter-element boundaries. Unavoidably, this leads to some non-local effects that extend beyond the boundaries between the three material phases. This is a simplification that may need further attention in future studies. Furthermore, at present the internal length of the ITZ is relatively large, which was necessary to avoid the need for extremely fine meshes and excessive computer times.

2.2. Numerical tests

The finite element method is used to simulate the response of the sample discretised with three-noded triangular elements. Each of the finite elements is assigned its own material properties corresponding to one of the three phases (see Table 1). The sizes of the elements have been chosen accordingly to the length-scale parameter: the matrix element size has been taken three times as small as the length-scale parameter. The size of the ITZ elements were chosen smaller than the size of the matrix elements in order to capture the curvature of the crack in the neighbourhood of an inclusion. The size of the elements in the inclusions has been taken much larger in order to save computer time, bearing in mind the fact that cracks cannot propagate through the inclusion (see the properties table below, crack initiation strain has been chosen artificially high).

Tension tests (Fig. 4) have been performed for the series of samples. Both periodic boundary conditions and periodicity of material are employed (Fig. 5). Below this terminology is explained in detail.

- *Periodicity of boundary conditions* refers here to a specific mesh construction, where nodes on the top and on the bottom borders of the sample identically repeat their positioning before and after the deformation (the same applies to the nodes on the left and right borders, Fig. 5 – left). This behaviour is implemented via penalty functions.

Table 2
Material components properties

Materials components properties	Inclusions	Matrix	ITZ
Crack initiation strain, [–], κ_0	0.5	5.0e−06	3.0e−06
Length-scale parameter [mm], ℓ	0.63	0.63	0.63

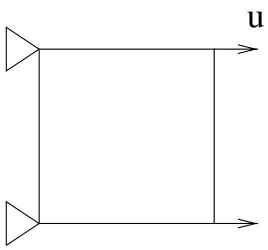

Fig. 4. Tension test.

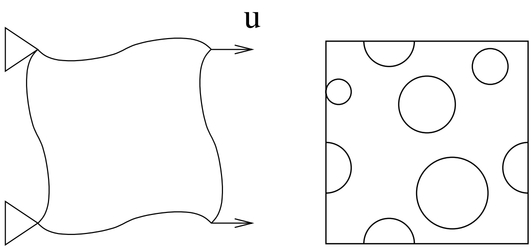

Fig. 5. Left: periodic boundary conditions; right: material periodicity (no wall-effect).

- *Periodicity of material* is understood here as a material experiencing no *wall-effects* (Fig. 5 – right). The term *wall-effect* refers here the inability of inclusions to *penetrate* through the sample borders. The motivation of using a *no-wall-effect* concept is that an RVE is thought of as belonging to a larger sample, therefore wall-effect is not a realistic representation. According to the definition, an RVE is first of all a *representative* volume. Thus it should *represent* any part of the material. In Fig. 6 several different situations have been displayed: samples A, B, D and E are valid in the context of periodicity of material. Although there are no inclusions crossing the edges in sample B, this should be considered a coincidence. On the contrary, the samples C and F are experiencing wall-effects: there are one or more edges which can not be crossed by inclusions. In this paper, wall-effects are avoided by allowing inclusions to penetrate through the sample borders and also by letting them re-appear through the opposite edge (see also [41]). As such, *periodicity of the material* is obtained (Fig. 7).

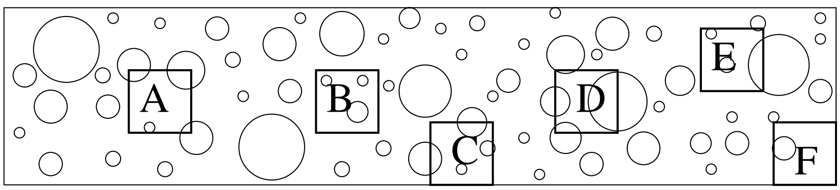

Fig. 6. Wall effect.

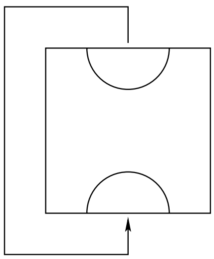

Fig. 7. Avoiding wall-effects by invoking periodicity of the material.

3. RVE existence: statistical analysis

With the assumption of periodicity of boundary conditions and material periodicity, the tension tests can be performed. As a result of the aforementioned tests, the load–displacement curves have been obtained first. The next step was to transform these curves into stress–strain curves. The stresses were obtained from the forces through a division by the cross-sectional area (here, as the two dimensional plain strain model is considered the cross-section areas were $L \times 1$, where L is the length of the particular tested specimen); and the strains are found from the displacements divided by the specimen size L. The stress–strain relations are shown in Fig. 8.

Each graph consists of one randomly chosen realisation of the four tested sample sizes. Three pictures correspond to three different volume fractions of inclusions, respectively.

The case of 30% of inclusions is presented further in more detail (Fig. 9). Four pictures, corresponding to four different sizes are plotted, each of them showing all five different realisations. Note, that the same analysis of different realisations has been performed for volume fractions 45% and 60%, and although they are not shown here the results of these analyses were qualitatively similar.

A statistical analysis, based on the mathematical expectation and standard deviation values, has been performed on each set of results. All curves (Figs. 8 and 9) were analysed in several points, corresponding to elastic, hardening and softening regions (Fig. 10) with stiffness (slope) being the parameter of interest. Hardening here denotes the nonlinear part of the pre-peak stress–strain curve. The choice of the stiffness as a parameter of interest could be explained by its relevance in multi-scale methods [17,26,27]. The stiffness is the quantity that is "up-scaled", i.e. transferred back to the macro-level. As such the value of stiffness is extremely relevant in homogenisation techniques. Strictly speaking, also the value of stress should be taken into account while considering the multi-scale procedure, however this is beyond the scope of the present paper. The information about stress-based RVEs can be found in [19].

Although the conclusion could be drawn from Fig. 9, that with increasing RVE size the difference in the slope values of different realisations is decreasing, i.e. the distance between the curves is getting smaller,

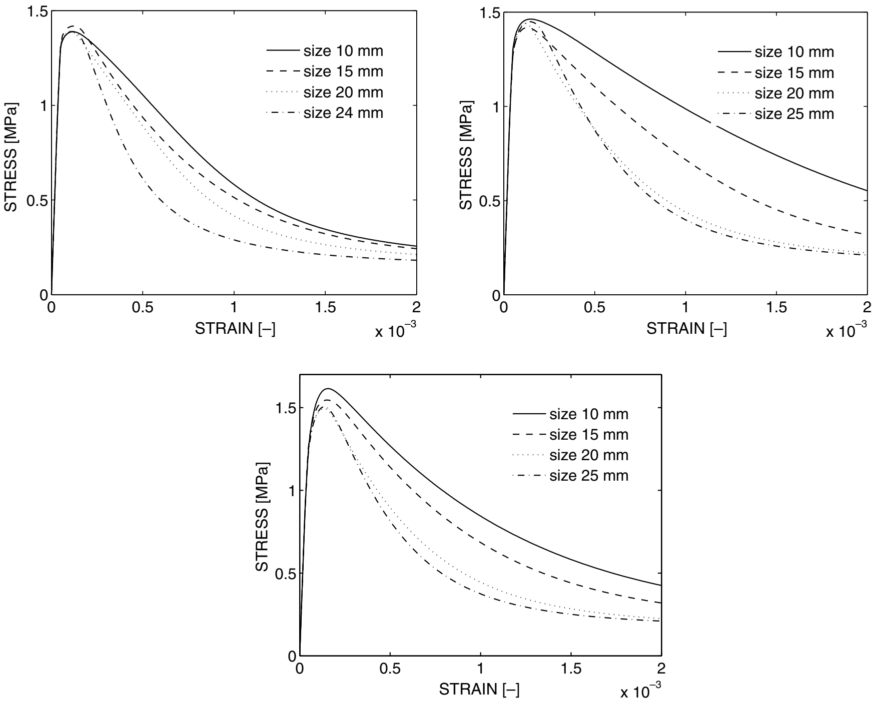

Fig. 8. Sets of sample sizes for volume fractions 30%, 45% and 60%.

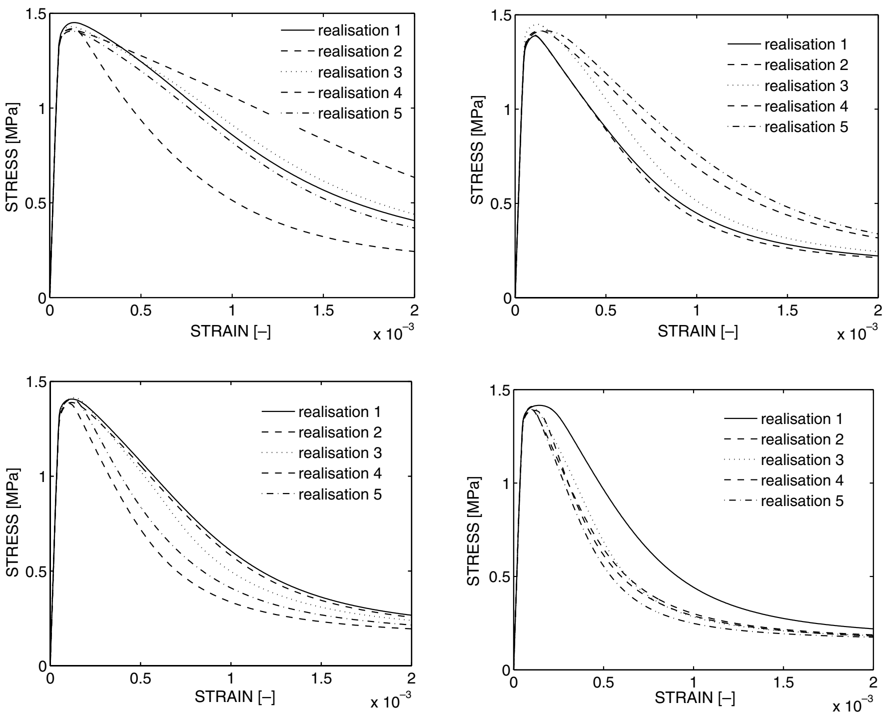

Fig. 9. Different sizes of the sample, from left to right and from top to bottom 10×10 mm^2; 15×15 mm^2; 20×20 mm^2; 25×25 mm^2 ($\rho = 30\%$).

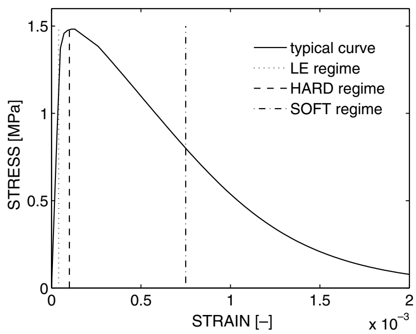

Fig. 10. Typical curve: linear-elastic, hardening and softening regimes.

Fig. 8 changes the picture: with increasing the size the slope becomes steeper. Fig. 11 offers a better understanding of the situation. The three regimes presented in Fig. 11 are linear-elastic (Fig. 11a), hardening (Fig. 11b) and softening (Fig. 11c). All curves (Figs. 8 and 9) are analysed by means of the mathematical expectation and standard deviation of the stiffnesses (value of slopes) in points corresponding to the three different regimes. In the linear-elastic case (Fig. 11a), the value of mathematical expectation (i.e. *average slope*) is practically constant with increasing size, and the standard deviation (i.e. *shifting of the slope from its average*) also converges to a constant value with increasing size. Material in hardening (Fig. 11b) shows the same trend: relatively constant mathematical expectation as well as standard deviation as size is increased. On the contrary, when in the softening regime (Fig. 11c), the standard deviation behaves qualitatively similar to linear elasticity and hardening (convergence with respect to size), but the mathematical expectation steadily increases (it should be noted, that here all values are considered as absolute). In other words, with increasing size, the material behaves differently (here, more brittle).

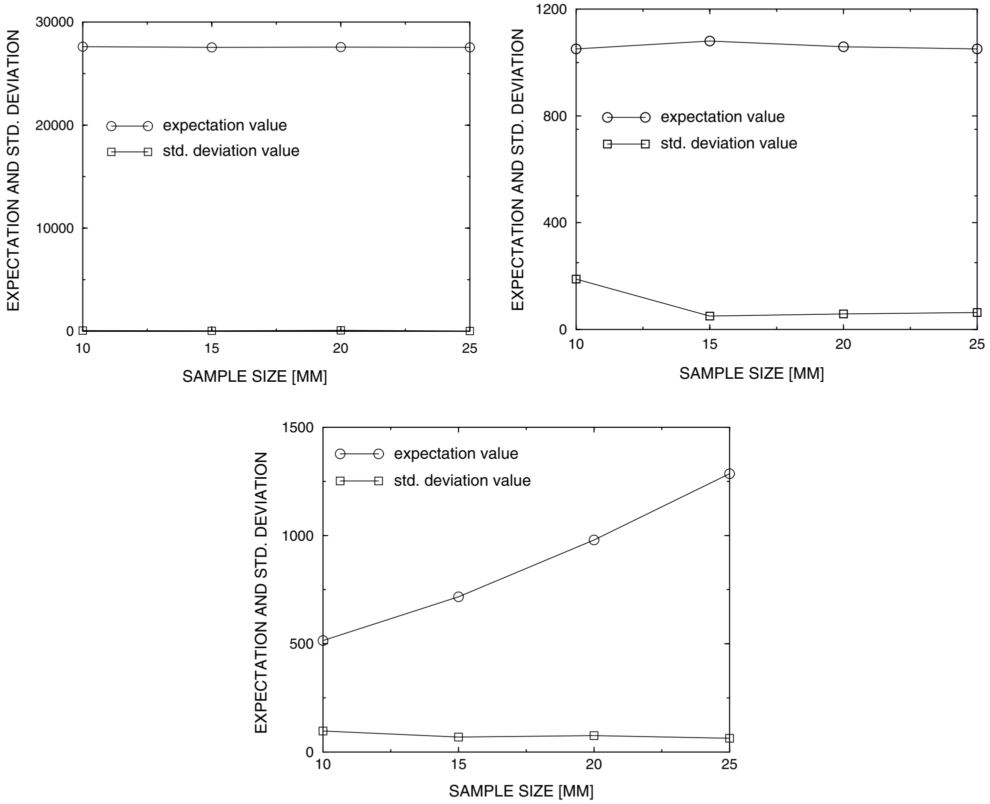

Fig. 11. Expectation and standard deviation values for different regimes: linear elasticity (left) hardening (right) and softening (the bottom).

Table 3
RVE existence

Results	Pre-peak	Post-peak
Convergence of expectation	+	–
Convergence of standard deviation	+	+
RVE existence	+	–

This statistical analysis allows to make a conclusion about RVE existence. In the pre-peak regime, the mathematical expectation shows a constant behaviour with respect to size while the standard deviation converges with increasing size. Therefore, representative volumes can be found. Conversely, in softening the mathematical expectation of the material stiffness does not converge with the specimen size, in other words, every size exhibits as intrinsically different material behaviour, and in conclusion an RVE cannot be found. This is summarised in Table 3.

4. RVE existence versus deterministic size effect

As it was mentioned above, the statistical analysis of a series of samples in softening showed that the response of the material qualitatively changes with increasing size (Fig. 11 – bottom: expectation values). The phenomenon that the response of a specimen changes with increasing size is also known as the *size effect* (see [51–53,2,3,7,10,13,25,47] among others). The extension of the deterministic size effect theory to the class of materials with explicitly defined inclusions and matrix is discussed below.

The deterministic size effect [2,3,7,13] can be caused by:

- different material overall properties due to the ratio between the structural size and the fracture zone, and/or
- the influence of the boundary [13].

Here, we treat deterministic size effects in terms of dissipated energy.

The results presented in Fig. 12 show the dissipated energy values in case of a tension test. The three curves describe a linear fit between different realisations corresponding to different sample sizes for volume fractions of inclusions equal to 30% (Fig. 12 – top left), 45% (Fig. 12 – top right) and 60% (Fig. 12 – bottom). The value of the dissipated energy has been evaluated as the area under the stress–strain curves. As it follows from the graph, the dissipated energy is decreasing with respect to increasing sample size. The value of the slopes in the logarithmic coordinates are very close to each other and approximately equal to -1, which corresponds to an inverse proportionality of the dissipated energy with the sample size. This inverse proportionality towards the size can be explained as follows:

- The localisation zone has a constant width (say w) independent of the sample size;
- The stored elastic energy is proportional to L^2;
- The energy necessary to create the localisation zone is proportional to $w \cdot L$;
- As a result, the ratio of dissipated (necessary) energy and elastic (available) energy is proportional to w/L;
- Consequently, the dissipated energy scales with $1/L$.

These trends are also observed in Fig. 8, and are caused by the localised solution for the sample.

Generally speaking, whenever the occurrence of a size effect is observed, the effects of statistical and deterministic size effects should be distinguished. The deterministic size effect has been discussed above in terms of dissipated energy, but a statistical size effect is also present in terms of strength. The strength of a specimen is largely determined by the stress concentration factors that occur upon loading. Stress concentration factors

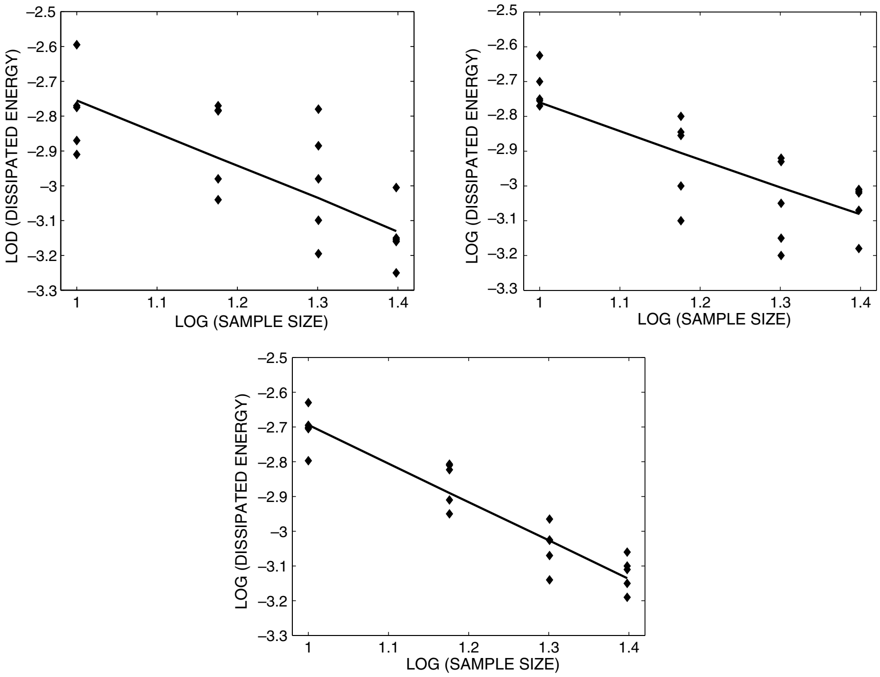

Fig. 12. Energy based deterministic size effect. Least-square fit for volume fracture 30% (top left), 45% (top right) and 60% (bottom).

increase in the neighbourhood of an inclusion, more so if this inclusion is relatively large, and even more so if two large inclusions are close to one another. A statistical size effect thus appears as a result of increasing the probability of the "weakest link" [51–53]: the larger the sample, the higher the probability of two large inclusions in contact, and therefore the higher the probability of failure initiation. Therefore, this statistical size effect relates to a *strength* size effect.

However, the statistical strength size effect is not related to the lack of RVE existence, since the strength size effect is related to the *peak* of the stress–strain diagram whereas the RVE ceases to exist *after the peak* in the stress–strain diagram. On the other hand, the considered deterministic size effect has been derived in terms of *dissipated energy*, and it therefore concerns the entire stress–strain diagram. The issue of the RVE non-existence for softening materials is confirmed by the existence of a deterministic size effect. It should be realised, however, that this argument may not be inversed: absence of any size effect does not imply existence of an RVE.

5. RVE size determination in the pre-peak regime

Once the question of an RVE *existence* is verified, and if it is positively answered, its *size determination* is the next issue to address.

In literature the concept of a representative volume element (RVE) was introduced to correlate the effective or macroscopic properties of materials with the properties of the microscopic constituents and microscopic structures of the materials. However, today little quantitative knowledge is available about minimum RVE sizes of various engineering materials. Several attempts have been made in order to determine the size of an RVE. For instance, [29] suggested that the three-dimensional RVE size should roughly be 0.1 mm for metallic materials, 1 mm for polymers, 10 mm for woods and 100 mm for concrete. In other studies, the RVE size for the hydraulic behaviour of gneissic rock was found as large as 12 m [50].

The general point of view is to connect the size of a representative volume of the heterogeneous material to the size of inclusions (reinforcements, grains, etc.). Van Mier and van Vliet in their experiments with concrete, for example, suggest the size of the RVE to be approximately equal to at least 3–5 times [45,48] or 7–8 times [46] the largest inclusion or particle size. In [4] it was proposed to take the size of the representative volume $V = \ell^{n_\mathrm{d}}$ where n_d is the number of spatial dimensions and ℓ the characteristic length of the material, which equals 2.7–3.0 times the maximum inclusion size [5,6].

Refs. [35,36] introduced a definition of minimum RVE size based on the concept of a nominal modulus, and determining numerically the minimum RVE sizes of more than 500 cubic polycrystals in the plane stress problem, under the assumption that all grains in a polycrystal have the same square shape (simple polycrystal model). They found that the minimum RVE sizes for effective elastic moduli have a roughly linear dependence on crystal anisotropy degrees. According to [35] with an error of 5% almost all of the tested materials have an RVE size of 20 or less times as large as the grain size. Together with a large overview of existing determined RVE sizes for different material types, [15] suggested that the minimum RVE contains in general 10 grains, though for the special case of stick-slip analysis they proposed to use an RVE containing at least 10^7 grains. On the other extreme of the range, Drugan and Willis derived for reinforced elastic composites the minimum RVE size to be equal to only twice the reinforcement diameter [12].

While most researchers relate the RVE size to the dimensions of the inclusions, the various suggestions for the RVE size in terms of the inclusion size differ by at least two orders of magnitude. Other parameters play a role in the quantification of the RVE size, such as for instance the volume fraction of the inclusions or the difference in stiffness between inclusions and matrix material. To assess the influence of these and other parameters, a closer look at the various quantification procedures should be taken.

5.1. RVE based on effective properties: numerical–statistical approaches

A number of approaches have been suggested in literature to analyse the RVE size numerically. They normally use multiple realisations for the meso-level sample, a finite element simulation of the samples and a statistical procedure to analyse the results. A typical example is provided by [24], whose methodology can be summarised as follows:

- generate different realisations of the microstructure for 4–5 different sample sizes;
- submit each microstructure to loading conditions and, for instance, periodic boundary conditions, and record the obtained effective properties;
- compute mean value and variance of effective property for the considered volume sizes;
- set the desired precision for the estimation of effective property and a number of realisations; use the model to define the final RVE size.

Other numerical–statistical approaches based upon setting a tolerance for the scatter in the results are given by [49,1]. A refinement to these approaches was proposed by [14]: an RVE will be the minimum volume, whose characteristics fluctuate in an *uncorrelated manner* and from which one is able to describe the macroscopic quantities and their fluctuations from its distribution characteristics.

Related to the above approach is the use of Monte–Carlo simulations. The idea of [31] was to consider Hooke's law as being either controllable by strains or stresses, and to check for which sizes the two responses begin to coincide. His method requires an explicit computational mechanics solution of a number of realisations of possible microstructures, sampled in a Monte–Carlo sense, which in turn allows a determination of statistics of both bounds. In a follow-up work [32] the stiffness difference between inclusions and matrix as well as the aspect ratio of the inclusions were varied. It was shown that with inclusion stiffness decreasing and their slenderness growing, the RVE tends to be very large. Ref. [21] generated statistically independent realisations of a periodic elastic composite with a disordered unit cell made up of 8, 27, and 64 non-overlapping identical spheres, after which Monte–Carlo runs were employed. By construction, all studied Monte–Carlo realisations had the same inclusion fraction. The overall elastic constants of these periodic Monte–Carlo realisations were then calculated numerically. It appears that the scatter in the individual elastic constants obtained with a few dozen spheres in the disordered unit cell is already remarkably small. The averages obtained with varying numbers of spheres are practically stationary. Thus, according to [21] based on only a few Monte–Carlo realisations, one can accurately predict the overall elastic constants of the studied periodic composite.

5.2. RVE based on effective properties: analytical approach

An estimation of the RVE size can also be done analytically. Ref. [12] employed an explicit non-local constitutive equation. They consider averaged strain fields that vary with position, and determine at which wave-length this variation will cause the non-local term in the constitutive equation to produce a non-negligible correction to the local term. On the basis of that they made an estimate of a minimum RVE size. They obtained quantitative results for the type of composite for which it is possible to render the non-local constitutive equation completely explicit: namely, two-phase composites consisting of an isotropic matrix reinforced (or weakened) by a random dispersion of isotropic spherical particles. Analytically derived explicit expressions were obtained for the RVE sizes in tensile and shear loading cases. The results of the study allowed to estimate the size of the RVE as approximately two times as large as the particle diameters for any reinforcement concentration level with high accuracy (95%). With exceptionally high accuracy (99%) they were able to show the RVE size to be approximately as large as 4.5 times the particle diameter.

5.3. RVE based on experimental observations

There have been many attempts to define the size of an RVE experimentally. Experimental analysis often involves selection of a particular sample geometry for mechanical testing and subjecting the specimen to image analysis after testing is complete. It is often assumed that the test specimen is representative of the material under investigation, but as it was mentioned by [20] this may only be determined by examining the length scale of fluctuations in heterogeneous entities which control the material response. In order to obtain meaningful results, a sufficient number of particles or volume of material must be included in both experimental and image analysis.

A methodology has been developed by [38] to arrive at a sufficiently small micro-structural size that can be referred to as an RVE of a non-uniform micro-structure of a ceramic matrix composite (CMC) containing a range of fibre sizes, and fibre-rich and -poor regions at the length scale of about 100 μm. Their RVE contains about 250 fibres of 14 μm diameter average size. The absolute size of the RVE is 0.1 mm^2. The proposed [38] methodology involves

- a combination of quantitative characterisation of geometry and spatial arrangement of micro-structural features using stereological and image analysis techniques;
- development of a computer model of the micro-structure that is statistically similar to the real micro-structure;
- numerical simulations of micro-mechanical response on computer-simulated microstructural windows of different sizes containing 60–2000 fibres;
- numerical simulations on large-area high-resolution digital image of the composite micro-structure containing about 2000 fibres.

The RVE has a micro-structure that is statistically similar to that of the CMC having fibre-rich and -poor regions. The Young's modulus of this RVE is very close to the Young's modulus of the composite. The modelled RVE has a local stress distribution that is comparable to that in the real composite under similar loading conditions.

Ref. [37] presented a theoretical background on the statistical requirements for an RVE. An image analysis technique using X-ray tomography was used to determine the RVE by measuring the volume at which the aggregate percentage becomes independent of the size of the volume analysed and reaches a constant value. The aggregate percentage was derived from different areas of two-dimensional images of asphaltic concrete.

Ref. [20] mentioned one other length scale dependent phenomenon. They have noticed, that defining an RVE of the material after damage and/or localisation of deformation has occurred is not straightforward; an RVE may even not exist. Nevertheless, some attempts were made to construct a representative volume in the presence of softening and damage. Although there were trials both numerically [28,42] and experimentally [20] to estimate such a representative volume, the conclusions were not promising. Extending their work from the class of elastic materials [43] to damaging material [42] it was concluded that the representative size of the microstructure is continuously increasing with evolving damage which makes it of little use in homogenisation schemes. Moreover, a softening material is developing a localisation zone and thus loses its statistical homogeneity. According to the RVE definition, an RVE cannot be found if statistical homogeneity is lost.

5.4. Suggested method to determine the RVE size

Combined numerical–statistical methods offer a good balance between general applicability on the one hand and the possibility of automated testing of different samples. For this reason, a combined numerical–statistical approach is chosen in this study to determine the RVE size. Similar to the numerical–statistical methods discussed above, different realisations are subjected to mechanical loading and their effective response is measured. In addition to determining mean and standard deviation, also the coefficient of variation and the Chi-square (χ^2) values are computed so that the statistical scatter can be compared objectively against a user-prescribed accuracy. The approach based on the Chi-square test is detailed in Fig. 13 and reads as a sequence of steps:

1. Fix the maximum and minimum diameters of inclusions and the initial size of the sample (usually two times as large as the maximum diameter of inclusions).
2. For the tested volume fraction of inclusions several (minimum 5) realisations of the tested sample size are generated.
3. Perform the finite element computation and present the results in the form of either load/displacement or stress/strain curve (dependent on the parameter of interest).
4. Perform the statistical analysis (see below for details) of the obtained finite element results.
5. Compare the accuracy of the statistical analysis results with the desired accuracy and if the obtained accuracy is good enough the tested sample size is the RVE size; otherwise increase the sample size and go to 3.

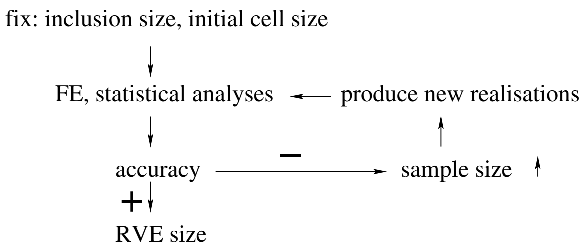

Fig. 13. RVE size determination procedure. Block scheme.

This procedure can be repeated for different materials, e.g. for different volume fractions or different material parameters.

Finding the variation coefficient as the ratio of the standard deviation to the mathematical expectation, it can be verified how the response of the single tested sample deviates relatively from the mean of its class of realisations. As a refinement, the effects of the deviation can be emphasized be taking its *square*. The latter method is known as *Chi-square test* or *Chi-square criterion*. This criterion reads

$$\chi^2 = \sum_{i=1}^{n} \frac{(a_i - \langle a \rangle)^2}{\langle a \rangle} \tag{4}$$

where a_i is the investigated parameter normalised with respect to its mean, $\langle a \rangle$ is the average of a_i in all samples, and n is the number of realisations, i.e. there are n samples with the same size, same volume fraction of inclusions but different inclusion distribution. Specifically, we have generated five samples for each volume fraction of inclusions and each sample size (see for instance Fig. 2). The investigated sizes of the sample range from $10 \times 10\ \text{mm}^2$ to $25 \times 25\ \text{mm}^2$ (see Fig. 1) and the dimensions of the inclusions follow a normal distribution from [2.5 mm to 5.0 mm]. In this paper the investigated parameter a_i is the average stress of the sample, although other parameters are also possible (cf. [40]). For a given volume fraction of inclusions the statistical analysis, based on the Chi-square criterion, gives the results presented in Fig. 14.

Now, with a desired accuracy of 95% and the statistical degree of freedom equal to 2 it is possible to find the table value of the Chi-square coefficient as 0.103. Plotting this table value together with experimentally obtained values of the Chi-square coefficients for different volume fraction of inclusions, it is possible now to find the corresponding size of the unit cell as an intersection of the experimental curves and the table value (Fig. 14 – left). This size of the sample will be considered as the size of the RVE with a given value of volume fraction of inclusions.

The next step of the procedure is to make a graph, corresponding to the value of the RVE for any types of material, i.e. for different volume fractions of inclusions (Fig. 14 – right). These results allow to find the size of the RVE with given volume fraction of inclusions of the material and accuracy. Corresponding values of the

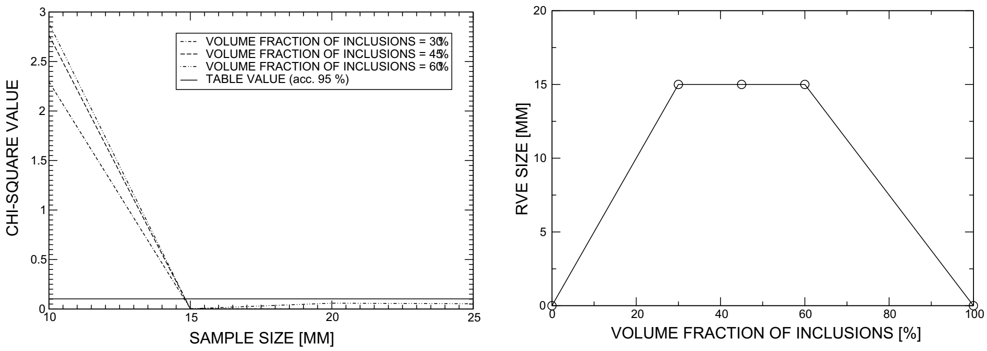

Fig. 14. Tension test (accuracy 95%): Chi-square values (left) with the table RVE size versus volume fraction of inclusion (right).

RVE for all different volume fractions of inclusions ρ are 15×15 mm^2, except the theoretical values 0×0 mm^2 for $\rho = 0\%$ and $\rho = 100\%$ (purely homogeneous materials).

Note 1. As can be deduced from the data given above, the smallest sample that is tested has a dimension which is twice the size of the largest inclusion. This hypothesis is widely used in literature: [12,11] in their articles, working with elastic composites, derived quantitative estimates for the minimum RVE size, so they have shown that the minimum RVE size is twice the reinforcement diameter.

Note 2. It has been assumed that the size of the RVE, being actually a stochastic value, follows the normal distribution. The number of parameters in the normal distribution is 2: mathematical expectation and standard deviation; thus having performed five realisations for each size and each volume fraction, the number of degree of freedom = number of realisations − number of distribution parameters − 1 = 5 − 2 − 1 = 2.

Note 3. In order to improve the accuracy of the quantitative analysis, one should consider more intermediate sizes in between the sizes 10×10 mm^2 and 15×15 mm^2 in Fig. 14 – left. Similarly, the accuracy of Fig. 14 – right can be improved by considering more intermediate values of the volume fraction of inclusions.

6. Periodicity versus non-periodicity

In this section the issue of the periodicity and its influence on the final RVE size is discussed. As it was mentioned in Section 2, two types of periodicity are considered: periodicity of material in terms of the wall-effect and periodicity of boundary conditions (Fig. 5). The importance of both types of periodicity is addressed below.

6.1. Periodic material

First, the material without wall-effect versus material with wall-effect have been tested. Periodic boundary conditions have been employed in both cases. Here it should be mentioned, that in order to analyse the periodicity issue in more detail not only tension but also shear tests have been performed. As it will be shown next, a different type of periodicity is more dominant under different loading schemes.

The results for the tension test are presented in Fig. 15 – left. A stress-based RVE denotes that the stresses are used in Eq. (4). As it can be verified, in case of the tension test the difference in RVE sizes is not extremely large compared to the following shear test results (see below).

For the case of shear loading materials with and without wall-effect have also been compared. The results of the shear test in case of no wall-effect and existence of wall-effect (i.e. material periodicity versus material non-periodicity) are presented in Fig. 15 – right. The shear test of the material with wall-effect shows that a reasonably accurate RVE size should be much larger than the maximum tested size of 25×25 mm^2. As it follows from Fig. 15 – right, the only possible RVE sizes for the non-periodic material in case of a shear test was found

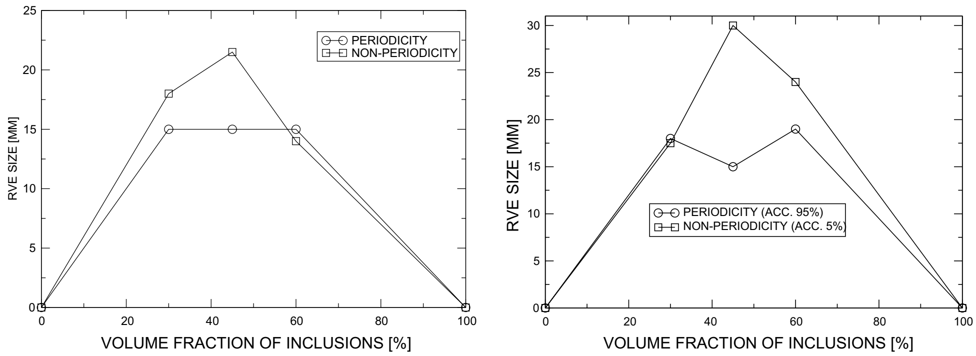

Fig. 15. Tension test (left) and shear test (right). Stress-based RVEs for material without wall-effect versus material with wall-effect; periodic boundary conditions are applied. Note the large discrepancy in accuracy for the shear test.

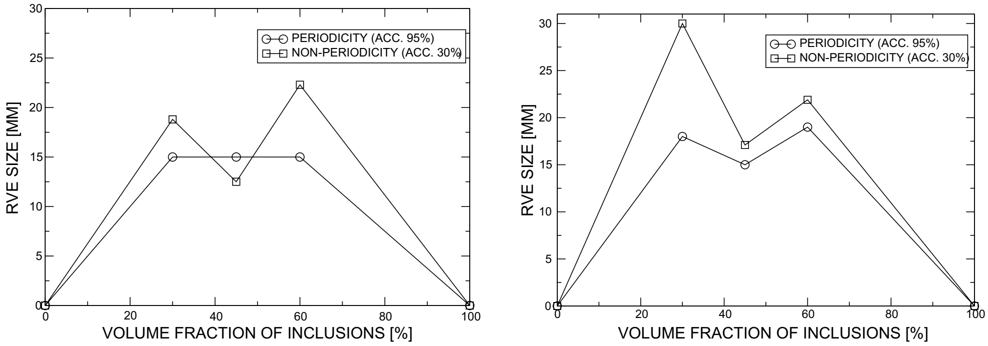

Fig. 16. Tension test (left) and shear test (right). Stress-based RVEs for material without wall-effect: periodic boundary conditions versus non-periodic boundary conditions.

with an unacceptable low accuracy of 5% (i.e. 95% error). Increasing the accuracy to levels comparable with the no wall-effect tests will lead to extremely large RVE sizes, which have not been generated in this study.

This brings us to the conclusion that in case of the tension test it is desirable but not essential to have material without wall-effect, but in case of shear test the absence of wall-effect is essential in order to describe realistic behaviour of the material. To understand the above observation one may think of a tension test in terms of prescribed deformations (for example horizontal stretching). In this case the restrained lateral deformation and the developed two normal stress components do not depend on particles penetrating (or not) the boundaries. Thus the issue of the material periodicity is not very essential in the tension case. On the contrary in case of shear, one could think of the test in terms of stiffnesses. Material without wall-effect guarantees that opposite sides of a specimen have more or less identical stiffnesses, however in case of material with wall-effect this is not necessary the case. As a result the scatter in the responses (and thus the RVE size) in case of non-periodic material is much larger than the one in the periodic material.

6.2. *Periodic boundary conditions*

Next the issue of periodic boundary conditions versus non-periodic boundary conditions has been analysed. Now periodicity of material is prescribed, i.e. the material without wall-effect is considered. Results show that for both tension (Fig. 16 – left) and shear (Fig. 16 – right) tests the RVE size should be extremely large (much larger than $25 \times 25\ \mathrm{mm}^2$ – maximum size tested) once accuracy of 95% is required. Note that a much lower accuracy of 30% had to be employed. Higher prescribed accuracy would lead to much larger sizes of the RVE in both tension and shear cases.

7. Conclusions

The representative volume concept, being widely used in mechanics, has been given a closer look in two aspects: first of all the question of an RVE *overall existence* has been worked out, and where proven to exist the RVE *size* has been determined next. Three regimes of material behaviour have been considered: linear elasticity, hardening and softening. Based on a statistical analysis the conclusions have been made about an RVE existence in these regimes. It appeared that an RVE can be found in both linear-elastic and hardening regimes. However, in the case of hardening the value of the standard deviation relative to the expectation is much larger than in linear-elasticity, which indicates that the size of the RVE in hardening is significantly larger than in linear-elasticity. It can be concluded comparing Fig. 11a and b: the deviation of the slopes in case of hardening is larger than in linear elasticity, in particular this is noticeable for small sizes of the sample. But once in softening, material loses the "representative" properties, in other words an RVE cannot be found. This is caused by the fact that the material in softening shows localisation. Material with such a localised behaviour loses statistical homogeneity. However an RVE can be found only for statistically homogeneous materials. Supporting the conclusion of an RVE non-existence in the softening regime, the size effect theory shows a strong deterministic size effect. These results have implications for the use of RVEs in for instance multi-scale analysis, in which lower scale (say meso-scale or micro-scale) analyses are embedded within an analysis on the higher scale (say the macro-scale). In case an RVE does not exist, special measures must be taken in order for such multi-scale methods to maintain their objectivity with respect to sample cell size. A particular solution to this problem has been suggested in [16] by introducing coupled-volume approach, whereby the sample cell size of the lower scale is related to the finite element size on the higher scale.

Next, attention has been given to the RVE size determination. The case of linear elasticity has been considered in detail. A procedure based on the Chi-square criterion has been presented in order to determine an RVE size. The size of the RVE in case of linear-elasticity has been found for the material in the tension test. The sensitivity of the RVE size to the periodicity in material configuration and boundary conditions in case of tension and shear loading schemes have been discussed. Two different types of periodicity have been analysed – periodicity of material in terms of wall-effect and periodicity of boundary conditions. The results show that for the tension test the periodicity of boundary conditions influences the results drastically: the size of the RVE in the case of non-periodic boundary conditions is much larger than the RVE size for the material with periodic boundary conditions. On the contrary, RVE sizes for material with and without wall-effect are relatively similar. For the shear test results, the conclusion is opposite: the material periodicity seems to be more dominant than periodicity of boundary conditions.

References

[1] Ashihmin VN, Povyshev IA. Statistical regularities of stress distribution in polycrystals. Math Model Syst Process 1995;3:11–8 [in Russian].

[2] Bažant ZP. Size effect. Int J Solids Struct 2000;37:69–80.

[3] Bažant ZP. Probabilistic modeling of quasibrittle fracture and size effect. In: Corotis, editor, Structural safety and reliability, 2001.

[4] Bažant ZP, Novák D. Stochastic models for deformation and failure of quasibrittle structures: recent advances and new directions. In: Bićanić N, de Borst R, Mang H, Meschke G, editors, Computational Modelling of Concrete Structures, 2003.

[5] Bažant ZP, Oh BH. Crack band theory for fracture of concrete. Mater Struct RILEM 1983;16:155–77.

[6] Bažant ZP, Pijaudier-Cabot G. Measurement of characteristic length of nonlocal continuum. J Engng Mech 1989;115(4):755–67.

[7] Bažant ZP, Yavari A. Is the cause of size effect on structural strength fractal or energetic–statistical? Engng Fract Mech 2005;72:1–31.

[8] Borbely A, Biermann H, Hartmann O. FE investigation of the effect of particle distribution on the uniaxial stress–strain behaviour of particulate reinforced metal-matrix composites. Mater Sci Engng A 2001;313:34–45.

[9] Bulsara VN, Talreja R, Qu J. Damage initiation under transverse loading of unidirectional composites with arbitrarily distributed fibers. Compos Sci Technol 1999;59:673–82.

[10] Carpinteri A, Chiaia B, Ferro G. Multifractal scaling law: an extensive application to nominal strength size effect of concrete structures. Politecnico di Torino, Torino, 1995.

[11] Drugan WJ. Micromechanics-based variational estimates for a higher-order nonlocal constitutive equation and optimal choice of moduli for elastic composites. J Mech Phys Solids 2000;48:1359–87.

[12] Drugan WJ, Willis JR. A micromechanics-based nonlocal constitutive equation and estimates of representative volume element size for elastic composites. J Mech Phys Solids 1996;44(4):497–524.

[13] Duan K, Hu X, Wittmann FH. Boundary effect on concrete fracture and non-constant fracture energy distribution. Engng Fract Mech 2003;70:2257–68.

[14] Evesque P. Fluctuations, correlations and representative elementary volume (REV) in granular materials. Poudres Grains 2000;11:6–17.

[15] Evesque P, Adjemian F. Stress fluctuations and macroscopic stick-slip in granular materials. Eur Phys J E 2002;9:253–9.

[16] Gitman IM. Representative volumes and multi-scale modelling of quasi-brittle materials. PhD thesis, Delft University of Technology, 2006. Available from <http://www.library.tudelft.nl/dissertations/>.

[17] Gitman IM, Askes H, and Sluys LJ. Representative volument size as a macroscopic length scale parameter. In: Li VC, Leung CKY, Willam KJ, Billington SL, editors, Fifth international conference on fracture mechanics of concrete and concrete structures, vol. 1, 2004, p. 483–91.

[18] Gitman IM, Askes H, Sluys LJ, Stroeven M. Multiscale modelling of granular materials. In: Bićanić N, de Borst R, Mang H, Meschke G, editors, Computational Modelling of Concrete Structures, 2003.

[19] Gitman IM, Gitman MB, Askes H. Quantification of stochastically stable representative volumes for random heterogeneous materialsauthor. Arch Appl Mech 2006;75:79–92.

[20] Graham S, Yang N. Representative volumes of materials based on microstructural statistics. Scripta Mater 2003;48:269–74.

[21] Gusev AA. Representative volume element size for elastic composites: a numerical study. J Mech Phys Solids 1997;45(9):1449–59.

[22] Hashin Z. Analysis of composite materials – a survey. J Appl Mech 1983;50:481–505.

[23] Hill R. Elastic properties of reinforced solids: some theoreticel principles. J Mech Phys Solids 1963;11:357–72.

[24] Kanit T, Forest S, Galliet I, Mounoury V, Jeulin D. Determination of the size of the representative volume element for random composites: statistical and numerical approach. Int J Solids Struct 2003;40:3647–79.

[25] Karihaloo BL. Size effect in shallow and deep notched quasi-brittle structures. Int J Fract 1999;95:379–90.
[26] Kouznetsova V, Brekelmans WAM, Baaijens FPT. An approach to micro–macro modeling of heterodeneous materials. Comput Mech 2001;27:37–48.
[27] Kouznetsova V, Geers MGD, Brekelmans WAM. Multi-scale constitutive modelling of heterogeneous materials with a gradient-enhanced computational homogenization scheme. Int J Numer Meth Engng 2002;54:1235–60.
[28] Lacy TE, McDowell DL, Talreja R. Gradient concept for evolution of damage. Mech Mater 1999;31:831–60.
[29] Lemaitre J. Continuum damage mechanics theory and applications. Wien-New York: Springer; 1987.
[30] Lemaitre J, Chaboche J-L. Mechanics of solid materials. Cambridge: Cambridge University Press; 1990.
[31] Ostoja-Starzewski M. Random field models of heterogeneous materials. Int J Solids Struct 1998;35:2429–55.
[32] Ostoja-Starzewski M. Scale effects in materials with random distributions of needles and cracks. Mech Mater 1999;31:883–93.
[33] Ostoja-Starzewski M. Microstructural randomness versus representative volume element in thermomechanics. ASME J Appl Mech 2002;69:25–35.
[34] Peerlings RHJ. Enhanced damage modelling for fracture and fatigue. PhD thesis, Technical University Eindhoven, 1999.
[35] Ren Z-Y, Zheng Q-S. A quantitative study of minimum size of representative volume elements of cubic polycrystals – numerical experiments. J Mech Phys Solids 2002;50:881–93.
[36] Ren Z-Y, Zheng Q-S. Effects of grain sizes, shapes, and distribution on minimum sizes of representative volume elements of cubic polycrystals. Mech Mater 2004;36:1217–29.
[37] Romero P, Masad E. Relationship between the representative volume element and mechanical properties of asphalt concrete. J Mater Civil Engng 1999;13:77–84.
[38] Shan Z, Gokhale AM. Representative volume element for non-uniform micro-structure. Comput Mater Sci 2002;24:361–79.
[39] Simone A. Continuous–discontinuous modelling of failure. PhD thesis, Delft University of Technology, 2003.
[40] Stroeven M, Askes H, Suys LJ. Numerical determination of representative volumes for granular materials. Comput Meth Appl Mech Engng 2004;193:3221–38.
[41] Stroeven P, Stroeven M. Assessment of packing characteristics by computer simulation. Cement Concr Res 1999;29:1201–6.
[42] Swaminathan S, Ghosh S. Statistically equivalent representative volume elements for unidirectional composite microstructures: Part II – with interfacial debonding. Cement Concr Res 2005;40(7):605–21.
[43] Swaminathan S, Ghosh S, Pagano NJ. Statistically equivalent representative volume elements for unidirectional composite microstructures: Part I – without damage. J Compos Mater 2005;40(7):583–604.
[44] Trusov PV, Keller IE. The theory of constitutive relations. Part I. Perm: Perm State Technical University; 1997 [in Russian].
[45] van Mier JGM. Fracture processes of concrete. USA: CRC Press, Inc.; 1997.
[46] van Mier JGM. Microstructural effects on fracture scaling in concrete, rock and ice. In: IUTAM symposium on scaling laws in ice mechanics and ice dynamics, 2000.
[47] van Mier JGM. Reality behind fictitious crack? In: Li VC, Leung CKY, Willam KJ, Billington SL, editors, Fifth international conference on fracture mechanics of concrete and concrete structures, vol. 1. 2004. p. 11–30.
[48] van Vliet MRA. Size effect in tensile fracture of concrete and rock. PhD thesis, Delft University of Technology, 2000.
[49] Vinogradov O. On a representative volume in the micromechanics of particulate composites. Mech Compos Mater 2001;37:245–50.
[50] Wang M, Kulatilake PHSW, Um J, Narviz J. Estimation pf rev size and three-dimensional hydraulic conductivity tensor for a fracturesd rock mass through a single well packer test and discrete fracture fluid flow modeling. Int J Rock Mech Mining Sci 2002;39:887–904.
[51] Weibull W. A statistical theory of the strength of materials. Stockholm: Royal Technical University; 1939.
[52] Weibull W. A statistical representation of fatigue failures in solids. In: Royal institute of technology, vol. 27, 1949.
[53] Weibull W. A statistical distribution function of wide applicability. J Appl Mech 1951:293–7.