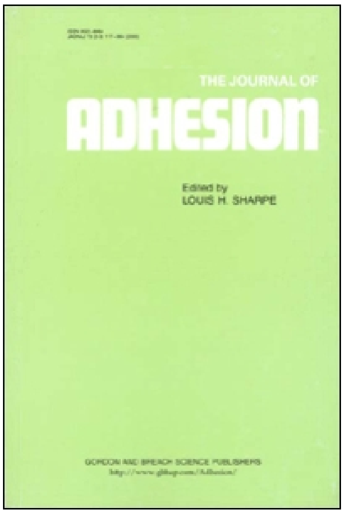

The Journal of Adhesion
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713453635

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To cite this Article Moshev, V. V. , Golotina, L. A. and Garishin, O. C.(1998) 'Continuum Models for Damageable Particulate Composites Based on Structural Formulations', The Journal of Adhesion, 65: 1, 207 — 216
To link to this Article: DOI: 10.1080/00218469808012246
URL: http://dx.doi.org/10.1080/00218469808012246

J. Adhesion, 1998, Vol. 65, pp. 207–216
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Continuum Models for Damageable Particulate Composites Based on Structural Formulations*

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(Received 30 November 1996; In final form 20 May 1997)

The method of transforming discrete structural models of particulate composites into adequate continuous representations is offered. Three dimensional levels of structural damage are treated as those of the cells, the finite elements and the specimens.

Keywords: Damageable particulate composites; continuum model; cell model; structural inhomogeneity; finite element method

1. INTRODUCTION

Recently [1] a rather abstract modeling of macrocrack formation from randomly-scattered microdamage initiated by deformation has been offered. In this approach, the material properties of a body are represented by a finite element system, where mechanical properties of finite elements vary within some definite range reflecting structural nonuniformity of particulate composites.

The mechanical behavior of individual finite elements is represented by means of some basic discrete model whose geometry has the form of a set of "cross-sections" tied in series. Each cross-section is composed of two rigid clamps interconnected in parallel by a number of

*One of a Collection of papers honoring Yuri S. Lipatov on the occasion of his 70th birthday, 10 July 1997.

elastic links that are primary structural elements of the system under consideration. As a whole, this structure is like a chain of elastic poker chips. The nonuniformity is introduced into the system through the nonuniformity of its primary elements, *i.e.* links, whose rupture elongations are imposed as random values. During extension, some links are ruptured in a random fashion, simulating individual microdamage events.

The microdamage accumulation enhances the elastic longitudinal nonuniformity of the discrete model to the extent at which the structure loses its elastic stability and breaks down in the most compliant part. The tensile behavior of the discrete model is then identified with the tensile behavior of some continuous medium with a set of corresponding parameters that are assigned to a given finite element. In such a manner, a transition from the discrete representation to the continuous one is performed. Such a scheme permits us to follow the entire finite element life-cycle from the virgin state to final failure without appealing to the so-called strength criteria.

In the model referenced in [1], the imposed structural parameters were chosen rather arbitrarily on the basis of common sense. However, later on, a representative structural cell was developed [2] that opened the way to refine the description of the behavior of the basic structural element, the link, and thus to get a clearer insight into the inner mechanisms leading to the macroscopic behavior of particulate composites. The present paper describes the refined variant of the model and demonstrates its potentialities.

2. THEORETICAL BACKGROUND

2.1. Structural Cell Characterization

The unit cell used as a basis for model development and its typical tensile stress-strain curve are shown in Figure 1. From the solution of this boundary value problem [2] for such a loading, one obtains a set of parameters describing a rather complicated tensile resistance of the cell, f, as a function of its extension, e. Analytically it may be expressed as

$$f = \begin{cases} g_1 e & \text{at } e < e_a \\ g_2 e + (g_1 - g_2) e_a \exp(-c(e - e_a)) & \text{at } e_a < e < e_b \\ 0 & \text{at } e > e_b \end{cases} \qquad (1)$$

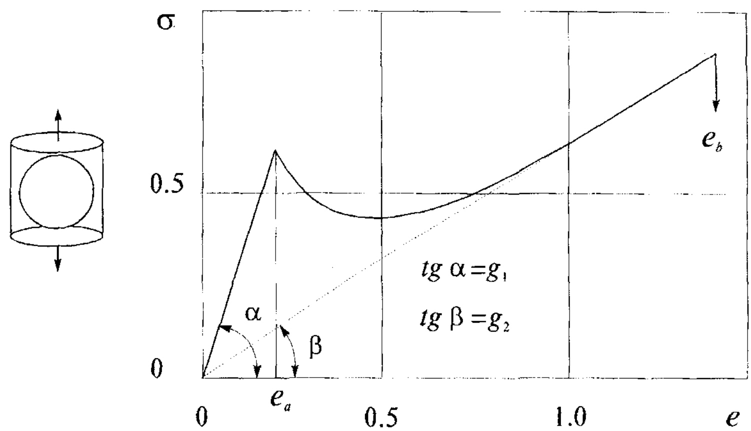

FIGURE 1 The shape of the unit cell and its typical tensile curve with specifying parameters.

Here g_1 and g_2 are the initial and final rigidities of the cell; e_a is the extension of the cell at which the separation of the matrix from the filler particle begins; e_b is the extension of the cell at which its breakdown occurs; and c is the parameter defining the span between the start and the end of the separation process. The magnitudes g_1 and g_2 are interrelated, both depending on the filler volume fraction, φ. This dependence of g_1 may be expressed as in Reference [3]

$$g_1 = E_m(1 + 1.25\,\varphi/(1 - \varphi/0.6))^2, \tag{2}$$

while g_2, according to our calculations, may be approximated as

$$g_2 = E_m(1 - 0.97\,\varphi^{0.54}), \tag{3}$$

where E_m is the Young's modulus of the matrix.

In References [4, 5], it was shown that internal tearing in elastomers occurs when the hydrostatic stress at the pole of the sphere reaches a magnitude equal to the Young's modulus of the matrix, E_m. Tearing the matrix at this place provokes its separation from the sphere. It has been assumed that this criterion may be regarded as the maximum achievable bond stress. Lesser magnitudes characterize adhesive debonds. In the following calculations maximum debond stress, σ_a, and accordingly debond strain, e_a, values taken from the boundary value solutions have been used.

After complete separation of the matrix from the filler particle, the strain concentration localized at the equatorial zone of the particle is characterized by the coefficient represented by the empirical formula

$$k = 1.5 + 6.53\,\varphi^3 + 2\,\varphi(1 - \exp(-4.5\,e)). \tag{4}$$

If the proper rupture deformation of the matrix is $(e_m)_b$ then the cell will finally be fractured at

$$e_b = (e_m)_b / k. \tag{5}$$

Thus, the mechanical behavior of the structural cell is now completely defined by the following basic structural parameters: filler volume fraction, φ, matrix modulus, E_m, matrix debond strain, e_a, and matrix breaking strain, $(e_m)_b$. The parameter c may be taken equal to 4.0 for all cases.

Hence, the tensile properties of the primary elements, the links, in the refined discrete model are now represented by Eq. (1) and accompanying Eq. (2)–(5).

2.2. Composite Structural Inhomogeneity

There exist at least two kinds of structural inhomogeneity: the geometrical local nonuniformity in the mutual arrangement of particles and the physical-chemical nonuniformity revealed as the debond nonuniformity.

The synthesis of the random geometrical structure consisting of identical spherical particles with the imposed filler volume fraction [6] allows one to obtain the scatters of the local matrix volumes surrounding filler particles that have the form shown in Figure 2. Analytical representation of these distributions has the general form

$$F(\varphi) = 1 - \exp(-\alpha\varphi^m)$$

where $F(\varphi)$ is the probability of encountering a φ smaller than the indicated one. From the above, it appears that the random character

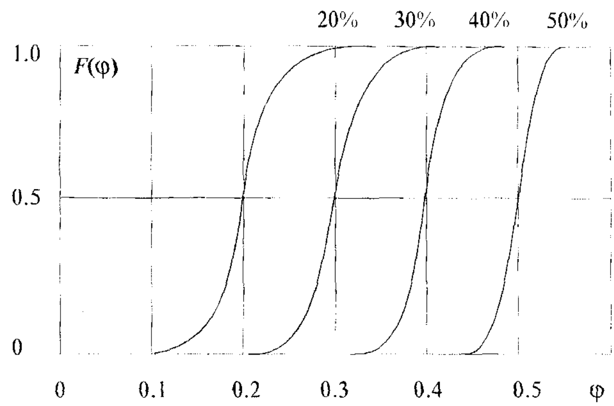

FIGURE 2 Integral distribution curves for local filler concentrations at various mean solid volume fractions indicated near the curves.

of φ induces the randomization of such cell parameters as g_1, g_2, e_a and e_b.

The determination of the scatter of the adhesive debond strains, e_a, caused not by geometrical stochasticity but by the physical-chemical local scatter, remains yet not feasible. In the subsequent text it will be ignored.

2.3. Finite Element Representation

The transformation of the discrete model into the continuous one can be accomplished through the utilization of the finite element approach. Evidently, it is impossible to treat the structure where one finite element is represented by one structural cell. Under such a condition, thousands (and possibly millions) of finite elements would have to be taken into account for adequate representation of realistic objects which goes far beyond the possibilities of modern computers. An averaging procedure seems to be inevitable. It may be realized by increasing the number of the cells that are to be enclosed in one finite element volume.

This may be performed in the following manner: first, one calculates the number of particles, N_c, within the volume of the specimen under consideration, having divided the total solid volume by the volume of one particle (obviously, filler concentration, particle size and specimen dimensions are to be imposed previously); second, discretization of the specimen volume into a grid of the finite elements is to be made and the total number, N_e, of finite elements within the volume of specimen is to be determined; third, having divided N_c by N_e, one finds the number of particles, n_{fe}, that are accounted for in one finite element.

Now the task is to evaluate the mechanical behavior of finite elements containing n_{fe} particles each. Identifying one particle and its surroundings with one structural cell, one gets a chance to use the above discrete model for the solution of this problem. This is done by assuming that the mechanical behavior of a finite element having n_{fe} particles is identical with that of a discrete model containing n_{fe} cells (links).

The calculated tensile curve of the discrete model represents an averaged tensile behavior of a given finite element. In the same manner, the averaged volume changes, based on summation of the volume changes of individual cells [7], are obtained. Typical views of the stress-strain and volume change-strain curves for a finite element holding 25 structural elements are shown in Figure 3.

The dependence of the modulus and volume changes on the deformation along the curve is then approximated up to the break-down point that is quite definite. The rupture occurs at the moment when the loss of the elastic stability of a finite element considered, induced by the damage accumulation, comes about. In calculations reported hereafter, finite elements containing hundreds of cells were used. The approach offered allows one to create a bridge linking discrete and continuous representations for damageable particulate composites.

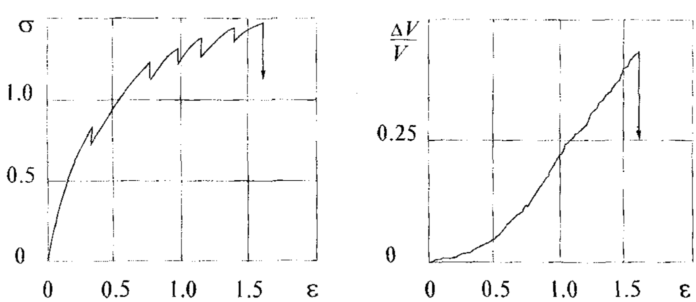

FIGURE 3 Typical dependencies of the shear modulus and volume changes as functions of deformation for an individual finite element.

2.4. Continuous Constitutive Relationships for Finite Element Representation

An isotropic Hookean elastic solid has been chosen as a constitutive continuous model for composites under consideration with the governing equations for the interconnection of stress, σ_{ij}, and strain, ε_{ij}, tensors as follows

$$\sigma_{ij} = 2G(\varepsilon_{ij} - \theta/3) + \delta_{ij}\sigma_0$$

where G is the current shear modulus, θ is the volume change, σ_0 is the mean stress, and δ_{ij} is the Kronecker delta.

The magnitude of G is found as a function of ε from the corresponding averaged relation for each finite element. The damage accumulation in continuous modeling is reflected through the ever-decreasing elastic modulus. It is assumed that in the 3-D conditions the value of G is determined by the value of the maximum main deformation, ε_1, that is assumed to be a parameter controlling the softening of the composite. Obviously, due to the stochastic nature of the composite material such relationships vary from one finite element to another.

In a similar fashion, the volume change for 3-D conditions also may be taken as a function of the maximum main deformation, ε_1. In the first approximation θ depends on ε_1 as follows

$$\theta = c_1 \varepsilon_1^{c_2}$$

where c_1 and c_2 are material constants specified for every finite element.

2.5. Computation Procedure

There is no need to describe the well-known scheme of the finite element implementation. In our case, the specificity of the computation consists in accounting for the shear and bulk modulus drop with deformation including final complete fracture for every finite element.

As a result of the original finite element nonuniformity, a large-scale nonuniformity appears and increases during deformation of the specimen ending in the loss of the longitudinal elastic stability and the rupture in the most compliant part of the specimen.

So the approach offered describes the complete life-cycle of the material without reference to the so-called strength criteria.

3. INVESTIGATION OF THE INFLUENCE OF SOME STRUCTURAL PARAMETERS ON MACROSCOPIC BEHAVIOR OF PLANE RECTANGULAR SPECIMENS

To illustrate the capabilities of the approach under consideration, a composite with a matrix having solid particles of 36 μm in diameter, a Young modulus of 3.0 MPa and a breaking strain of 3.0 has been examined. The choice of parameters allowed the comparison to be made with the available experimental data.

The calculations were performed for solid volume fractions of 0.1, 0.2 and 0.3, the range for all the concentrations being adopted. Figure 4 (a) demonstrates the calculated stress-strain curves while Figure 4 (b) represents experimental data from Reference [8]. The similarity between both figures seems to be satisfactory. The calculated breaking strains and stresses of the composite specimens are about 3 times and 5 times smaller than those of the pure matrix.

The diminution of the particle sizes, obviously leading to higher uniformity of the material, should provide higher ultimate properties.

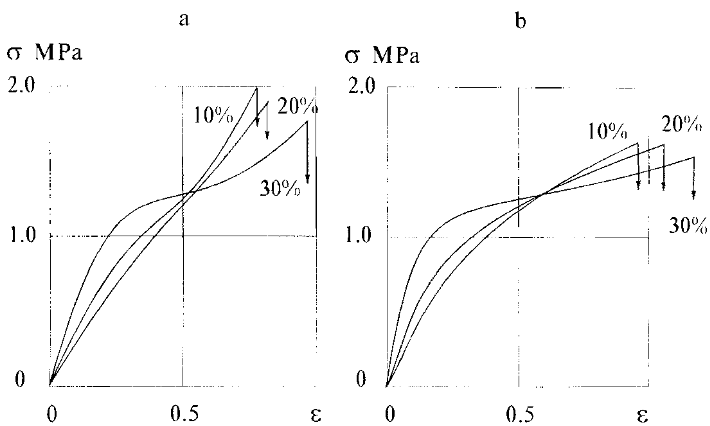

FIGURE 4 The calculated (a) and experimental (b) tensile curves. Numerical values near the curves indicate filler concentraiton.

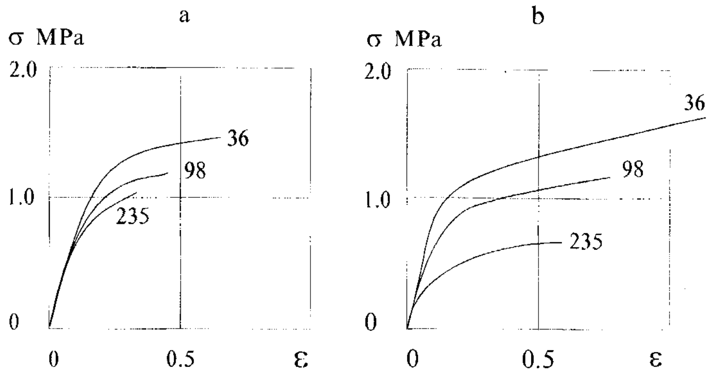

FIGURE 5 The effect of particle size on the tensile curves, (a) calculated, (b) experimental. Numerical values near the curves indicate filler particle sizes.

The influence of the particle sizes has been examined for particles of 36, 98 and 255 μm in diameter. The calculated and experimental [8] data are shown in Figures 5(a) and (b), respectively.

This figure, as a preceding one, demonstrates the qualitative similarity between calculated and test results.

4. CONCLUSION

A method of transforming discrete structural models of particulate composites into adequate continuous representations is offered.

Three-dimensional levels of structural damage are treated as those of the cells, the finite elements and the specimens.

The calculated and experimental data seems to be qualitatively similar to each other.

The approach offered should be regarded as a "breadboard" model requiring subsequent detailed exploration and refinement.

Acknowledgements

The research reported in this paper has been supported by the Russian Academy of Sciences under grant 94-01-00465.

References

[1] Moshev, V. V. and Golotina L. A., "Nonlinear mechanical models for particulate elastomeric composites. III. Macrocrack initiation from randomly scattered microdamages," *Ukrainian Polymer J.* **4** (1–2), 70–84 (1995).

[2] Moshev, V. V. and Kozhevnikova, L. L., "Unit cell evolution in structurally damageable particulate-filled elastomeric composites under simple extension," *J. Adhesion* **55**, 209–219 (1996).

[3] Chong, J. S., Christensen, E. B. and Baer, A., "Rheology of concentrated suspensions," *J. Appl. Polym. Sci.* **15**, 2007–2021 (1971).

[4] Gent, A. N. and Park, B., "Failure process in elastomer at or near a rigid spherical inclusion," *J. Mater. Sci.* **19**, 1947–1956 (1984).

[5] Oberth, A. E. and Bruenner, R. S., "Tear phenomena around solid inclusions in castable elastomers," *Trans. Soc. Rhebl.* **9**, 165–185 (1965).

[6] Moshev, V. V. and Garishin, O. K., "Physical discretization approach to evaluation of elastic moduli of highly filled granular composites," *Int. J. Solids Structures* **30**(17), 2347–2355 (1993).

[7] Moshev, V. V. and Kozhevnikova, L. L., "Pressure reinforcement of particulate polymeric composites originated by adhesive debonding," *J. Adhesion* **55**, 197–207 (1996).

[8] Schwarzl, F. R., Bree, H. W. and Nederveen, C. J., "Mechanical properties of highly filled elastomers. I. Relationship between filler characteristics, shear moduli, and tensile properties," *Proc. 4-th Intern. Congr. Rheology*, Vol. 3 (Interscience/Wiley, NY, 1965), pp. 241–263.