EFFECT OF FILLER AGGREGATES STRUCTURE ON COMPOSITE ELASTIC PROPERTIES.

V. G. Oshmyan, S. A. Patlazhan, S. A. Timan

Department of Polymer and Composite Materials, N.N. Semenov Institute of Chemical Physics, 4 Kosygin St., Moscow 117977, Russia.

SUMMARY: Elastic scaling behavior of a continuous anisotropic fractal, 2D Sierpinski carpet, is the subject of the study. In the case of porous in elastic matrix, P. Sheng and R. Tao [4] and S. A. Patlazhan [5] have found that axial and shear moduli of the carpet exhibit distinct scaling with the size of the system. However, it is widely accepted that different stiffness of isotropic fractals scale with equal exponents. The nature of such discrepancy has remained unclear. Using numerical position-space renormalization group technique, we show that different stiffness of the carpet also scale with equal exponents. In particular, it means that both in the cases of porous and rigid inclusions fractal Poisson ratio has non zero values independent of matrix moduli. Difference in the values of scaling exponents obtained in previous study is caused by analysis of the initial fractal generations.

KEYWORDS: elasticity, fractal, scaling, renormalization, disordered composite.

INTRODUCTION.

The elastic properties of isotropic fractal structures (regular or random) have been studied since 1984 [1-5]. In particular, it was shown [2,3] numerically in the framework of discrete spring-based models that stiffness C of rigid percolation clusters (random fractals) above the elasticity threshold exhibit power-law (scaling) behavior with the size L of the system: $C \propto L^{-\tau}$. Also, it is widely accepted that percolation clusters are isotropic fractals, and different components of effective stiffness tensor **C** scale with the same exponents.

P. Sheng and R. Tao [4] first investigated elastic scaling behavior of a continuous anisotropic regular fractal - the 2D Sierpinski carpet (Fig. 1). In the case of porous in an elastic matrix (*elastic problem*), calculation of effective moduli was based on an iterative solution of the Dyson equation for elastic wave scattering in a heterogeneous media. Due to the square symmetry of the carpet, three moduli determine tensor **C**. It was found that axial [8], C_{11}, $C_{11}-C_{12}$, and shear, C_{44}, moduli exhibit scaling behavior with corresponding exponents:

$$\tau_1 \approx 0.27, \quad \tau_2 \approx 0.25, \quad \tau_3 \approx 0.46\,. \tag{1}$$

Using different approach, S. A. Patlazhan [5] has obtained another estimates of the same exponents:

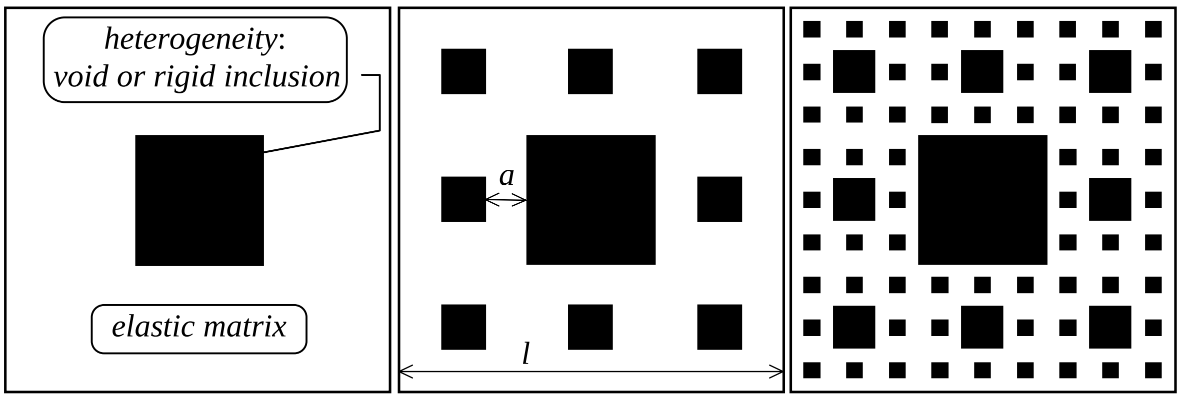
$$\tau_1 \approx 0.25, \quad \tau_2 \approx 0.26, \quad \tau_3 \approx 0.33 . \qquad (2)$$

In the case of rigid inclusions (*superelastic problem*), scaling law $C \propto L^s$ was found, but with equal exponents:

$$s_1 \approx s_2 \approx s_3 \approx 0.14 . \qquad (3)$$

It follows from qualitatively consisted estimates (1) and (2) that, contrary to the isotropic case, axial and shear moduli of the Sierpinski carpet exhibit *distinct* elastic scaling behavior. The nature of such discrepancy has remained unclear. However, it was proposed [4] two possible origins. The first one is in the square symmetry of the carpet. Another contributing factor may be the breakdown of analogy between the discrete and continuum elasticity.

Several important questions have arise from previous study. In both papers, linear $\log(C) - \log(L)$ dependencies were obtained for the three initial generations of the carpet under the unique value of the matrix Poisson ratio $\nu = 0.2$. However, the scaling elastic response should be expected at large L. Whether the same scaling would be asserted for the developed fractal structure? Would it be varied with the host parameters?



(a) $n=1$, $L=3$ **(b)** $n=2$, $L=9$ **(c)** $n=3$, $L=27$

Fig. 1.
The three initial generations of a Sierpinski carpet. The size L of the system is defined as the ratio of the side l of the outer square to the minimal thickness a of the matrix and is determined by the number n of the generation: $L = l/a = 3^n$.

Recently [6], we have computed tensor **C** for the three initial generations of the carpet numerically, using the finite element method (FEM). It was found that: (*i*) the exponents depend on ν; (*ii*) the linearity of $\log(C) - \log(L)$ dependencies is broken as matrix approaches to the limit of incompressible media with ν close to unity [9]. So, we must conclude that estimates (1) and (2) obtained for the initial fractal generations are determined by specific relations between matrix moduli and may be inconsistent at large L.

Unfortunately, direct FEM-based calculation is not applicable at large L because of computer memory and time consuming. Construction of the position-space renormalization group (PSRG) transformation and its application for analysis of scaling behavior of 2D Sierpinski carpet elastic moduli at large L is the subject of the paper. An idea of the PSRG transformation is in the substitution of effective moduli of a finite fractal generation back into the same generation as the matrix moduli. This procedure was suggested, but not performed in the paper [4]. To do this, effective matrix should be regarded as an elastic continuum complied with the same square symmetry as a finite generation of the carpet. If this condition is satisfied, the transformation can be iterated as far as necessary. Therefore, arbitrary size of the fractal can be analyzed. We have found that both for elastic and superelastic problems the PSRG transformation has corresponding stable fixed points, $\mathbf{P}_e^* = \left(\Sigma_e^*, A_e^*\right)$ and $\mathbf{P}_s^* = \left(\Sigma_s^*, A_s^*\right)$, on a plane of the effective Poisson ratio

$$\Sigma = C_{12} / C_{11} \tag{4}$$

and coefficient of anisotropy

$$A = \left(C_{11} - C_{12}\right) / \left(2C_{44}\right). \tag{5}$$

An existence of the finite fixed points provides a common scaling for different components of tensor **C** with exponents independent of matrix mechanical properties: $\tau \approx 0.29$ and $s \approx 0.17$.

The rest of the paper is organized as follows. The description of the PSRG transformation forms a content of the next section. The results of simulations are discussed in the final part of the paper.

PSRG TRANSFORMATION.

Let us define dimensionless size L of the system as a ratio of the side l of outer square to the minimum thickness a of the matrix (Fig.1). It is determined by the number n of the fractal generation:

$$L = l/a = 3^n. \tag{6}$$

Following the definition (6), the size of the homogeneous square without inclusions ($n = 0$) is equal to 1. So, we denote initial stiffness tensor of matrix as $\mathbf{C}(1)$.

The FEM code elaborated in the paper [6] under assumption of isotropic matrix ($A = 1$, independent C_{11} and C_{44}) was used for computation of components C_{11}, C_{12} and C_{44} of effective stiffness tensor $\mathbf{C}(L,\mathbf{C}(1))$ at $L = 3$, 9, 27 and 81. (Below, where it is not lead to ambiguity, the second argument will be dropped, i.e. $\mathbf{C}(L,\mathbf{C}(1)) = \mathbf{C}(L)$). In that case, we can define transformation $\mathbf{f}_n$ mapping matrix moduli on effective moduli of the nth fractal generation:

$$\mathbf{C}\left(3^n\right) = \mathbf{f}_n\left(\mathbf{C}(1)\right). \tag{7}$$

Unfortunately, the transformation (7) does not conserve the isotropy of **C** and thereby cannot be iterated. Generalization of the FEM code on a matrix complying with the square symmetry (independent C_{11}, C_{12} and C_{44}) allows us to define PSRG transformation $\mathbf{f}_n$ induced by the nth generation in the form suitable for iterations. :

$$\mathbf{C}\left(3^n L\right) = \mathbf{f}_n\left(\mathbf{C}(L)\right). \tag{8}$$

According to the definition (8), numerical PSRG technique consists in the following. Given arbitrary values of initial matrix moduli $C_{11}(1)$, $C_{12}(1)$ and $C_{44}(1)$, we apply the FEM code for computation $C_{11}(3^n)$, $C_{12}(3^n)$ and $C_{44}(3^n)$. Then we repeat computation of effective moduli of

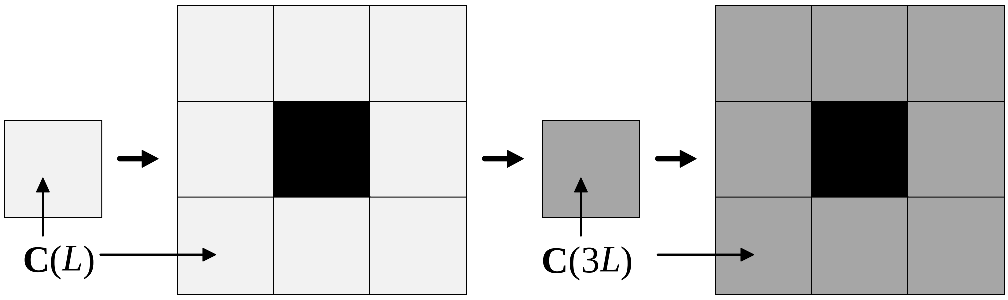


Fig. 2.
One step of the PSRG transformation (8) induced by the 1st fractal generation.

the nth fractal generation using the components of previously obtained tensor $\mathbf{C}(3^n)$ as the new matrix moduli. As a result, we obtain tensor $\mathbf{C}(9^n)$. This homogenization procedure may be continued until arbitrary preassigned value of L will be reached. After k iterations, tensor $\mathbf{C}(3^{nk})$ effectively accounts an influence of inclusions of the size less than $L = 3^{nk}$. A scheme of the procedure described is illustrated on Fig. 2 at $n = 1$.

Obviously, the result of the PSRG technique application should be dependent of the two parameters. Accuracy of numerical method is the first one. This factor can be excluded by the choice of sufficiently large FE mesh, which is supposed to be done. The second parameter is the level n of the transformation (8), which cannot be excluded and seems to be important. For example, $\mathbf{C}(9)$ can be approximated using maps $\mathbf{f}_1$:

$$\mathbf{C}(9) = \mathbf{f}_1\left(\mathbf{f}_1\left(\mathbf{C}(1)\right)\right), \tag{9}$$

or $\mathbf{f}_2$:

$$\mathbf{C}(9) = \mathbf{f}_2\left(\mathbf{C}(1)\right). \tag{10}$$

It is not a priori known whether the left sides of the Eqns. (9) and (10) are close to each other. This problem will be discussed in the next section on the basis of the numerical data obtained.

Due to the infinite ratio between stiffness of matrix and inclusions, right side of Eqn. (8) is a homogeneous function of order one for both elastic and superelastic fractals:

$$\mathbf{f}_n(\alpha\mathbf{C}) = \alpha\,\mathbf{f}_n(\mathbf{C}), \quad \text{for arbytrary real } \alpha. \tag{11}$$

Condition of homogeneity (11) and definitions (4) and (5) allow us to define reduced map $\mathbf{r}_n$ in a plane of the Poisson ratio Σ and coefficient of anisotropy A:

$$\begin{aligned} \Sigma(3^n L) &= (\mathbf{r}_n)_\Sigma\left(\Sigma(L), A(L)\right) \\ A(3^n L) &= (\mathbf{r}_n)_A\left(\Sigma(L), A(L)\right), \end{aligned} \tag{12}$$

where $(\mathbf{r}_n)_\Sigma$ and $(\mathbf{r}_n)_A$ are given throw components of the map $\mathbf{f}_n$:

$$(\mathbf{r}_n)_\Sigma = \frac{(\mathbf{f}_n)_{12}}{(\mathbf{f}_n)_{11}}, \qquad (\mathbf{r}_n)_A = \frac{(\mathbf{f}_n)_{11} - (\mathbf{f}_n)_{12}}{2(\mathbf{f}_n)_{44}}. \tag{13}$$

Existence of the finite fixed point $\left(\Sigma_n^*, A_n^*\right)$ of map (12):

$$\left(\Sigma_n^*, A_n^*\right) = \mathbf{r}_n\left(\Sigma_n^*, A_n^*\right), \quad \Sigma_n^* \neq 0,\infty \quad \text{and} \quad A_n^* \neq 0,\infty, \tag{14}$$

and equality $\left(\Sigma(1), A(1)\right) = \left(\Sigma_n^*, A_n^*\right)$ provide size independent stiffness ratios and exact scaling law for effective moduli:

$$C \propto L^{-\tau_n} \text{ or } C \propto L^{s_n}, \tag{15}$$

where the universal exponents τ_n and s_n are given by the formula:

$$\tau_n, s_n = \left|\frac{\lg\left(\left(\mathbf{f}_n\right)_{11}\left(\mathbf{C}_n^*\right)\right)}{n\lg 3}\right|, \tag{16}$$

and independent components of $\mathbf{C}_n^*$ are determined by stiffness ratios corresponding to the fixed point: $\left(\mathbf{C}_n^*\right)_{11} = 1$, $\left(\mathbf{C}_n^*\right)_{12} = \Sigma_n^*$, $\left(\mathbf{C}_n^*\right)_{44} = \left(1-\Sigma_n^*\right)/\left(2A_n^*\right)$.

It will be shown below that $\mathbf{r}_n$ is a contraction map. This implies convergence on (Σ, A) plane of the iterative procedure described above:

$$\mathbf{r}_n^k\left(\Sigma(1), A(1)\right) = \left(\Sigma(L), A(L)\right) \to \left(\Sigma_n^*, A_n^*\right), \quad k, L \to \infty, \tag{17}$$

and asymptotic validity of scaling law (15) for arbitrary initial matrix moduli.

RESULTS AND DISCUSSION.

Unique fixed point values $\left(\Sigma_n^*, A_n^*\right)$ of the $\mathbf{r}_n$ have been found for every tested level n. Obtained results are summarized in Table 1.

Table 1.

Fixed points of the map (12) and corresponding exponents (16).

Elastic fractal				
n	1	2	3	4
Σ^*	0.075	0.069	0.066	0.066
A^*	3.02	3.77	4.23	4.33
τ	0.298	0.296	0.291	0.284
Superelastic fractal				
n	1	2	3	4
Σ^*	0.103	0.085	0.075	0.064
A^*	2.42	2.97	3.33	3.70
s	0.176	0.170	0.168	0.169

Convergence (17) of the flow diagrams of iterated map $\mathbf{r}_n$ has been checked by numerical analysis in wide range of initial matrix values both for elastic (Fig. 3a) and superelastic (Fig. 3b) fractals.

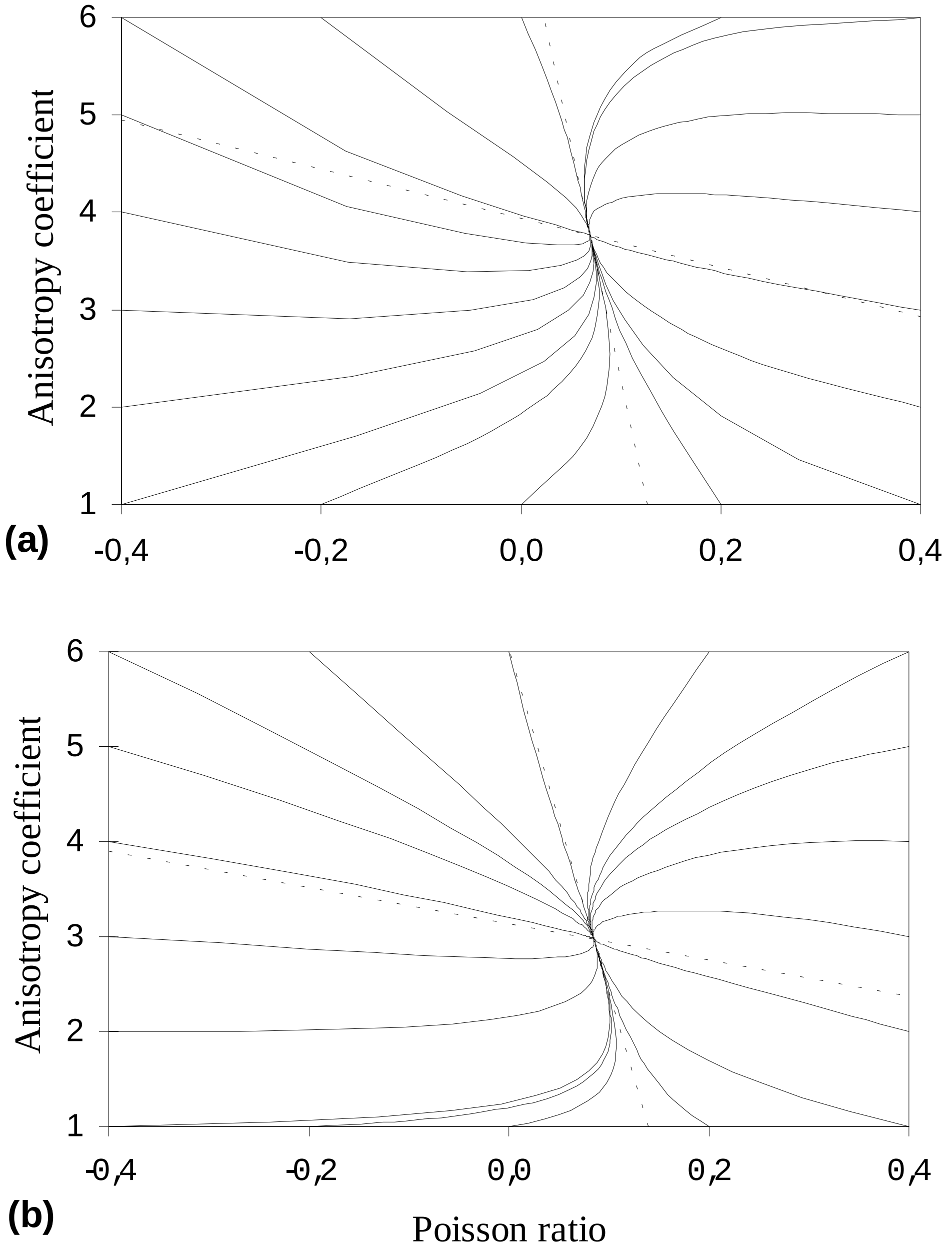


Fig. 3.

The flow diagrams of iterated maps $\mathbf{r}_2$ (12) (solid lines) for elasic (a) and superelastic (b) fractals and corresponding eigendirections of the linearized maps $\mathbf{R}_2$ (18) (dotted lines).

Near fixed point, contraction property of the $\mathbf{r}_n$ was directly proved by its linearization:

$$\mathbf{r}_n(\Sigma, A) - (\Sigma_n^*, A_n^*) \approx \mathbf{R}_n \begin{pmatrix} \Sigma - \Sigma_n^* \\ A - A_n^* \end{pmatrix}, \tag{18}$$

and computing of eigenvalues, λ_1, λ_2, and corresponding eigenvectors, $\mathbf{e}_1$, $\mathbf{e}_2$, of the linearized map $\mathbf{R}_n$. The results of the analysis for $n = 2$ (Fig. 3) are given in Table 2. It is seen from Fig. 3 and Table 2 that contraction condition $1 > |\lambda_1| \geq |\lambda_2|$ is satisfied and flow diagrams tend to the eigendirections corresponded to the maximum eigenvalues.

Table 2.

Eigenvalues, λ_1, λ_2, and eigenvectors, $\mathbf{e}_1$, $\mathbf{e}_2$, of linearized maps $\mathbf{R}_2$ (18) for elastic and superelastic fractals.

λ_1	$\mathbf{e}_1$	λ_2	$\mathbf{e}_2$
Elastic fractal			
0.76	(-0.02,1)	0.52	(0.37,-0.93)
Suprelastic fractal			
0.9	(-0.03,1)	0.8	(0.46,-0.89)

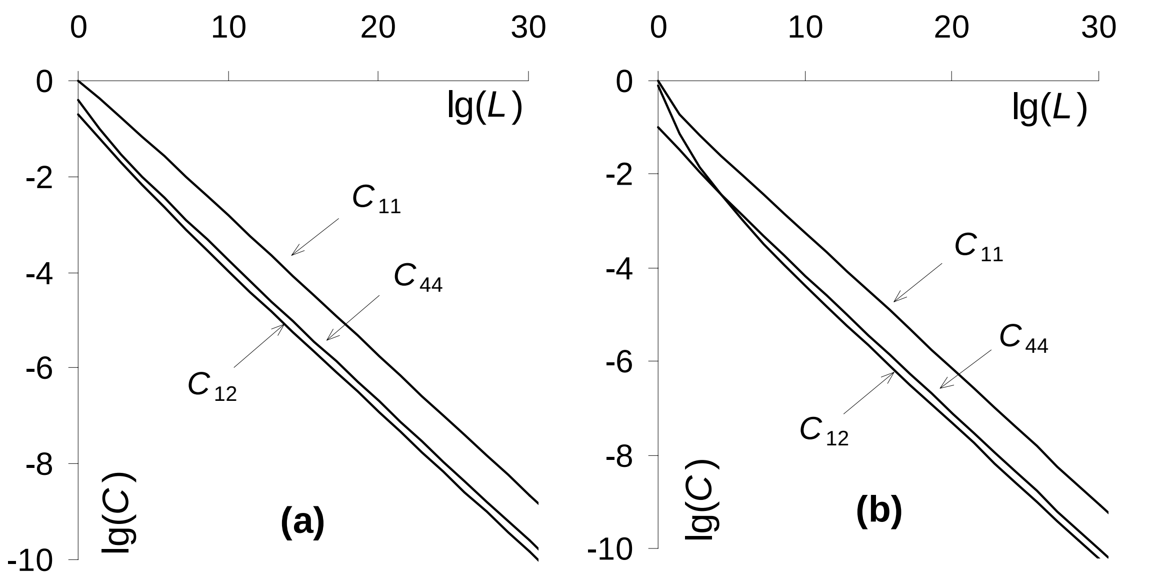


Fig. 4.

The log(C)–log(L) dependencies of elastic carpet. Matrix Poisson ratio $\Sigma(1)=0.2$ (a) and $\Sigma(1)=0.8$ (b). In both cases, matrix coefficient of anisotropy $A(1)=1$.

As it was already mentioned in the previous section, existence of the fixed point and contraction property of the $\mathbf{r}_n$ provide not only convergence (17) in the ratio plane, but also universal asymptotic scaling law (15). Validity of the last was directly checked by drawing of log(C)–log(L) plots (Fig. 4). It is interesting to note that linearity of the plots is almost valid in the hole range of the sizes including small ones in the case of $\Sigma(1)=0.2$, $A(1)=1$ (Fig. 4a). This feature was found and discussed in the first publications [4,5], concerning elastic scaling properties of the Sierpinski carpet of initial generations. However, linearity of the initial portions of the plots does not hold for $\Sigma(1)=0.8$, $A(1)=1$ (Fig. 4b). The reason of such difference is caused by the different distance from matrix values of the ratios to that of the fixed point, which is much less in the first case (see Fig. 3a). In particular, inequality $C_{44}>C_{12}$, which is a case of fixed point, holds for $\Sigma(1)=0.2$, but becomes opposite if the matrix becomes close to incompressible media.

Naturally, the limit $n \to \infty$, which corresponds to the infinitely developed fractal sets, is interesting. These limit have been estimated by 2-power polynomial approximation of the numerical data of Table 1 with respect to $\varepsilon = 1/n$ and $\varepsilon = 1/\lg(n)$ (Table 3). There is seen certain discrepancy between the estimates obtained by the different approximations. The data on larger iteration level n is necessary to define exponents more exactly. However, the

Table 3.
Estimates of scaling exponents and fixed point values for 2D Sierpinski carpet.

Elastic fractal			
Limit	τ	Σ^*_∞	A^*_∞
$\varepsilon = 1/n$	0.284	0.0651	4.43
$\varepsilon = 1/\lg(n)$	0.267	0.0621	5.06
Superelastic fractal			
Limit	s	Σ^*_∞	A^*_∞
$\varepsilon = 1/n$	0.168	0.063	3.74
$\varepsilon = 1/\lg(n)$	0.167	0.035	4.71

divergence is small, so data of Table 2 can be used as rough estimates.

It is attractive to assume that scaling properties of the fractal are primary determined by the dimension of the set and thereby to estimate the exponents for elastic and superelastic percolation problem on the basis of the results obtained for regular fractals. Let us use Sierpinski carpet as a model of percolation cluster for the speculation suggested. Size L of the system is related to the matrix volume fraction $p^{(m)}$ as $L^d/L^D = L^{(d-D)}$, where $d = \ln 8 / \ln 3$ and $D = 2$ be fractal and configurational dimensions, correspondingly. It is widely accepted that in the neighborhood of percolation threshold p_e elastic or superelastic behavior of highly disordered system is mainly determined by the properties of rigid or soft infinite cluster. If one supposes that fraction $p^{(m)}$ of the matrix in fractal is proportional to $\left|p - p_e\right|$, then elastic, T,

$$C \propto \left(p - p_e\right)^T \tag{19}$$

and superelastic, S,

$$C \propto \left(p_e - p\right)^{-S} \tag{20}$$

exponents can be estimated on the basis of the data of Table 3:

$$T \approx \frac{\tau}{D-d} \approx 2.55, \quad S \approx \frac{s}{D-d} \approx 1.5 \tag{21}$$

Sure, much more convincible arguments should be done to ground the estimates (21). However, the relation $T > S$, which holds [1-3,7] for 2D disordered elastic systems, is also supported by simulations on regular elastic and superelastic fractals - 2D Sierpinski carpet.

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8. Below, we use the accepted notations for components C_{ijkl} of tensor **C** in a 2D continuum of square symmetry: $C_{1111}=C_{2222}=C_{11}$, $C_{1122}=C_{12}$, $C_{1212}=C_{44}$.
9. Recall that Poisson ratio for 2D media takes values on the interval [-1,1]