Percolation Threshold for Elastic Problems: Self-consistent Approach and Padé Approximants

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Abstract

Self-consistent approximation and Padé approximants are used for calculation of percolation threshold for elasticity problem.

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1. Introduction

Mathematical models of composite materials can be rather complicated as a result of the distribution and orientation of the multiple inclusions within the matrix. Properties of inclusions are usually very different of properties of matrix. If the distribution of inclusions is completely random, then with an increase in their volume fraction c_2 the chains of the contacting inclusions (clusters) are created in the material. The critical value $c_2 = c_p$, for which the cluster of an infinite length is formed, is called the percolation threshold. The properties of such composite materials cannot be described within the framework of regular or quasi-regular models, and it is necessary to use the theory of percolation. This theory was intensively developed in the recent decades [1, 2, 3, 4, 5, 6, 7]. The objectives of the theory of percolation consist in description of the correlations between the appropriate physical and geometrical characteristics of the objects under study.

Effective characteristics k_0 of a composite near the percolation threshold ($c_2 \to c_p$) are defined by the asymptotic relations like

$$k_0 \sim |c_2 - c_p|^t, \tag{1}$$

where c_p is the critical volume fraction of the inclusions, t is the critical index of the corresponding physical property.

Different models of percolation media and corresponding methods of calculation of percolation threshold and the critical indices are reviewed in [1, 2, 3, 4, 5]. It is worth to note that until now there is a certain discrepancy between the results of different authors, especially in the 3D case.

For transport problems it is shown that Bruggeman's formula (self-consistent approximation) makes it possible to qualitatively describe the percolation threshold [2, 6, 7]. However, the accuracy of Bruggeman's formula is low. In the paper [6] a modification of Maxwell's formula is proposed based on the Padé approximant (PA), which provides a qualitative explanation of the existence of the percolation threshold.

In our paper we analyse using of self-consistent approximation and PA for calculation of percolation threshold for elasticity problem. Percolation threshold depends on the shape of inclusions. We will consider in the present paper the spherical inclusions in 3D case.

2. Self-consistent Approach

Well-known self-consistent approach [8, 9, 10] leads to the following equations for effective shear modulus μ^*, bulk modulus K^* and Poisson's coefficient ν^*:

$$\sum_{i=1}^{2} \frac{c_i}{1+\alpha^*\left(\frac{K_i}{K^*}-1\right)} = 1;\ \sum_{i=1}^{2} \frac{c_i}{1+\beta^*\left(\frac{\mu_i}{\mu^*}-1\right)} = 1;\ \nu^* = \frac{3K^*-2\mu^*}{6K^*+2\mu^*}, \qquad (2)$$

where

$$\alpha^* = \frac{1+\nu^*}{3\left(1-\nu^*\right)},\ \beta^* = \frac{2\left(4-5\nu^*\right)}{15\left(1-\nu^*\right)};$$

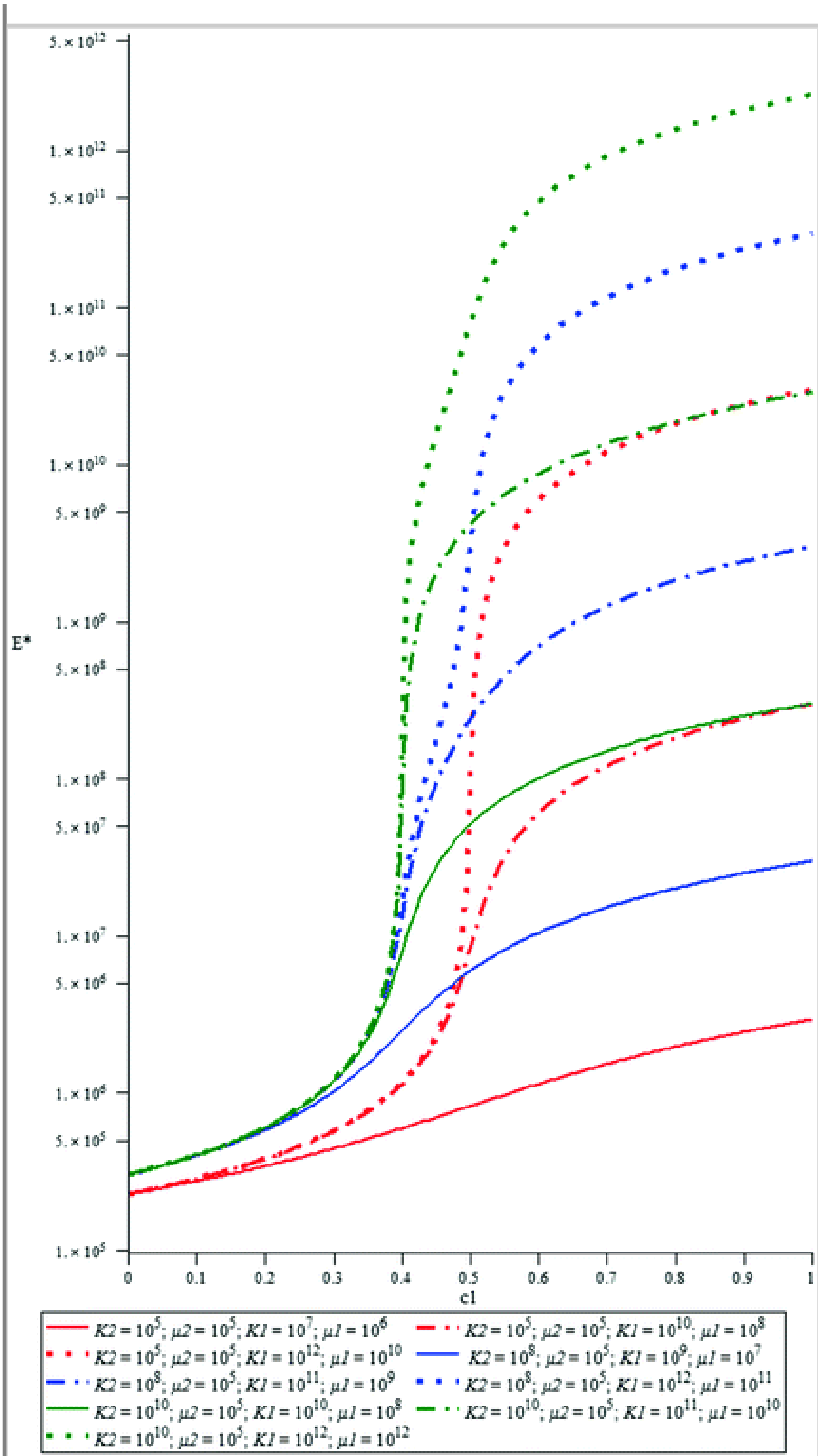
K_1, μ_1 and K_2, μ_2 are the elastic constants of inclusions and matrix respectively; $c_i\ (i=1,2)$ are the volume fractions, $c_1+c_2=1$.

The system of Eq. (2) admits an exact analytic solution (we do not give it due to its cumbersome nature), which allows us to obtain the expression for the effective Young's modulus E^*.

Figure 1 shows the graphs of the effective Young's modulus E^*, obtained due the solution of the system of Eq. (2), for various values of the elastic characteristics of the matrix K_2, μ_2, and inclusions K_1, μ_1.

Fig. 1

Graphs of the effective Young's modulus E^* for various values of the elastic characteristics of the matrix and inclusions



Analysis of these dependences shows that in the case of rigid inclusions, whose elastic characteristics significantly exceed the values of the corresponding parameters of the matrix ($K_1 \gg K_2$, $\mu_1 \gg \mu_2$), the self-consistency solution describes a qualitatively the percolation threshold in the composite material.

In particular, for the values of the elastic constants of the matrix $K_2 = 10^{10}$, $\mu_2 = 10^5$, and inclusions $K_1 = 10^{12}$, $\mu_1 = 10^{12}$, the percolation threshold obtained by the self-consistent approach agrees with the experimental data [11], where it is shown that for the composite with the mentioned elastic characteristics the percolation threshold is located between 0.40 and 0.41.

3. Padé Approximants for Virial Expansions

Virial expansions for effective shear μ^* and bulk K^* modulus at small inclusions concentrations can be written as follows [9, 12]:

$$K^* = \left[1 + \frac{3\left(1-\nu_2\right)\left(K_1 - K_2\right)c_1}{2K_2\left(1-2\nu_2\right) + K_1\left(1+\nu_2\right)}\right]K_2; \quad (3)$$

$$\mu^* = \left[1 + \frac{15\left(1-\nu_2\right)\left(\mu_1 - \mu_2\right)c_1}{\mu_2\left(7-5\nu_2\right) + 2\mu_1\left(4-5\nu_2\right)}\right]\mu_2. \quad (4)$$

Using well-known relations

$$E = \frac{9K\mu}{3K+\mu},\ \nu = \frac{1}{2}\cdot\frac{3K-2\mu}{3K+\mu},$$

and formulas (3), (4) one obtains effective Young's modulus E^*:

$$\begin{aligned} E^* = {} & \left[9\mu_2\left(4\mu_2^2\left(2-5c_1\right) + \mu_1\left(3K_2\left(3-5c_1\right) + 4\mu_1\left(3+5c_1\right)\right) + 5K_2\mu_1\left(2+3c_1\right)\right)\right. \\ & \left.\times\left(\mu_2\left(4K_2\left(1-c_1\right) + 4K_1c_1\right) + 3K_2\left(-K_2c_1 + K_1\left(1+c_1\right)\right)\right)\right]/\left[16\left(2-5c_1\right)\mu_2^4\right. \\ & + 4\left(3K_2\left(11-13c_1\right) + 3K_1\left(2+3c_1\right) + 4\mu_1\left(3+5c_1\right)\right)\mu_2^3 \\ & + 3\left(K_2\left(28\mu_1\left(2-c_1\right) + 3K_1\left(11+15c_1\right)\right) + 4K_1\mu_1\left(3+17c_1\right)\right)\mu_2^2 \\ & + 9K_2\left(K_2\left(4\mu_1\left(2-5c_1\right) + 9\left(K_1\left(1+c_1\right) - K_2c_1\right)\right) + K_1\mu_1\left(14+25c_1\right)\right)\mu_2 \\ & \left.+ 54K_2^2\mu_1\left(-K_2c_1 + K_1\left(1+c_1\right)\right)\right]. \end{aligned} \quad (5)$$

The range of applicability of the virial expansion ы method is limited by the small concentrations of one of the components; therefore, the relations (3)–(5) cannot be used for large inclusions and even at a qualitative level do not describe the percolation threshold. For improving formula (5) let us use PA [13]. PA $[0/1]$ for E^* is:

$$E^{*\,(0)}_{[0/1]}\left(c_1\right) = \frac{9K_2^2\mu_2\Delta_1^{(1)}}{K_2\left(3K_2+\mu_2\right)\Delta_1^{(1)} - \left(3K_2+4\mu_2\right)\Delta_2^{(1)}c_1}, \quad (6)$$

where

$$\begin{aligned} \Delta_1^{(1)} &= \left(3K_1+4\mu_2\right)\left(6K_2\mu_1 + 9K_2\mu_2 + 12\mu_1\mu_2 + 8\mu_2^2\right); \\ \Delta_2^{(1)} &= 45K_1K_2^2\left(\mu_1-\mu_2\right) + 3K_1K_2\mu_2\left(2\mu_1+3\mu_3\right) + 3K_2^2\mu_2\left(18\mu_1 - 23\mu_2\right) + \\ & \quad 4\left(K_1-K_2\right)\mu_2^2\left(3\mu_1+2\mu_2\right). \end{aligned}$$

Similarly, we construct a PA $[1/0]$ for the expression obtained from (5) by replacing: $K_{1(2)} \overset{\rightarrow}{\underset{\leftarrow}{}} K_{2(1)}$, $\mu_{1(2)} \overset{\rightarrow}{\underset{\leftarrow}{}} \mu_{2(1)}$, $c_1 \rightarrow c_2$. From the physical point of view, we reversed the roles of the phases of the composite "matrix"—"inclusion". In this case, the corresponding PA is written as:

$$E^{*\,(0)}_{[1/0]}\left(c_2\right) = \frac{9K_1\mu_1}{3K_1+\mu_1} + \frac{9\mu_1\left(3K_1+4\mu_1\right)\Delta_2^{(2)}}{\left(3K_1+\mu_1\right)^2\Delta_1^{(2)}}c_2, \quad (7)$$

where $\Delta_i^{(2)} = \Delta_i^{(1)}\ (i = 1, 2)$ after change: $K_{1(2)} \underset{\leftarrow}{\overset{\rightarrow}{}} K_{2(1)}$, $\mu_{1(2)} \underset{\leftarrow}{\overset{\rightarrow}{}} \mu_{2(1)}$.

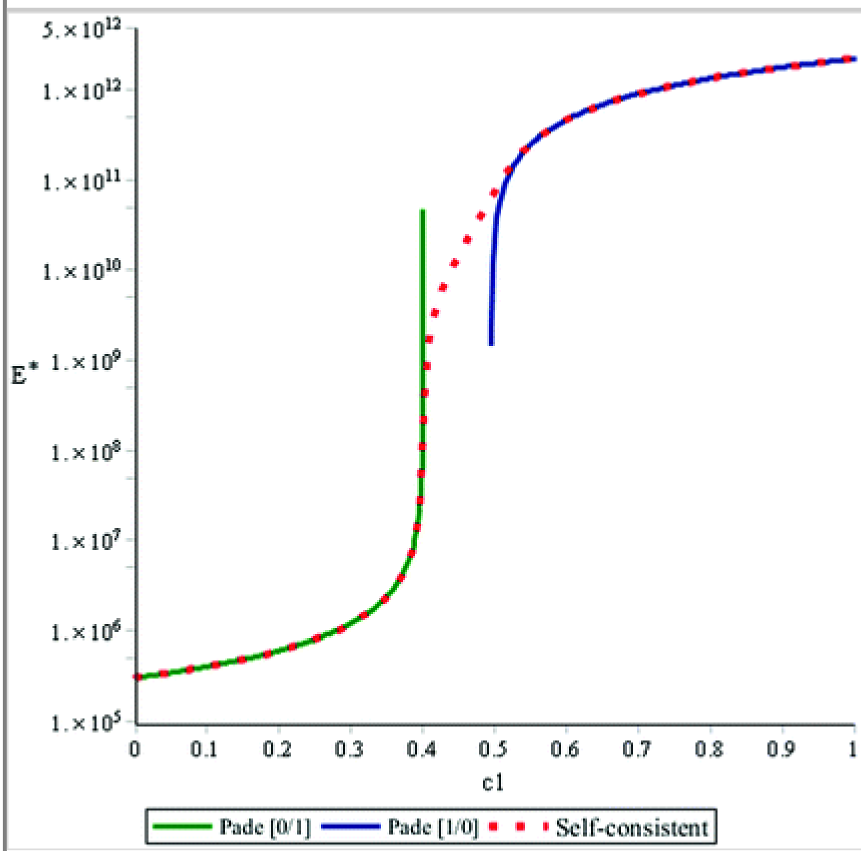
Passing in the Eq. (7) to the variable c_1 ($c_2 = 1 - c_1$), for $c_1 \to 1$ finally we have:

$$E^{*\,(1)}_{[1/0]}(c_1) = \frac{9\mu_1\left((3K_1+\mu_1)\left(K_1\Delta_1^{(2)}+\Delta_2^{(2)}\right)+\mu_1\Delta_2^{(2)}-(3K_1+4\mu_1)\,\Delta_2^{(2)}c_1\right)}{(3K_1+\mu_1)^2\Delta_1^{(2)}}. \quad 8$$

In Fig. 2 at the values of the elastic constants of the matrix material and inclusions: $K_1 = 10^{12};\ \mu_1 = 10^{12};\ K_2 = 10^{10};\ \mu_2 = 10^5$ graphs of the effective Young's modulus obtained using the self-consistency method (2) and using the Padé approximants (7), (8) are presented.

Fig. 2

Comparison of the results of calculations of the effective Young's modulus by self-consistent approach and PA of virial expansions



We can conclude that

i. the PA allows us to expand area of applicability of virial expansion substantially;

ii. a comparison with the self-consistent solution shows that the PA at zero (7) reliably describes the effective parameter right up to the percolation percolation threshold;

iii. the PA in unit (8) works well for large inclusions: the results practically coincide with the self-consistent solution.

To estimate the accuracy of the constructed PA, we use the Hill equation, which is an exact relation that does not depend on the microstructure of the composite. This equation is valid for composites consisting of isotropic components having the same shear modulus of components. For a two-dimensional two-component composite with $\mu_1 = \mu_2 = \mu$ this equation is written as:

$$\frac{1}{\mathrm{K}^* + \mu} = \frac{\mathrm{c}_1}{\mathrm{K}_1 + \mu} + \frac{\mathrm{c}_2}{\mathrm{K}_2 + \mu}, \tag{9}$$

from which the expression of an effective bulk modulus follows directly:

$$K_H^* = \frac{(c_1 K_1 + c_2 K_2)\ \mu + K_1 K_2}{c_1 K_2 + c_2 K_1 + \mu}. \tag{10}$$

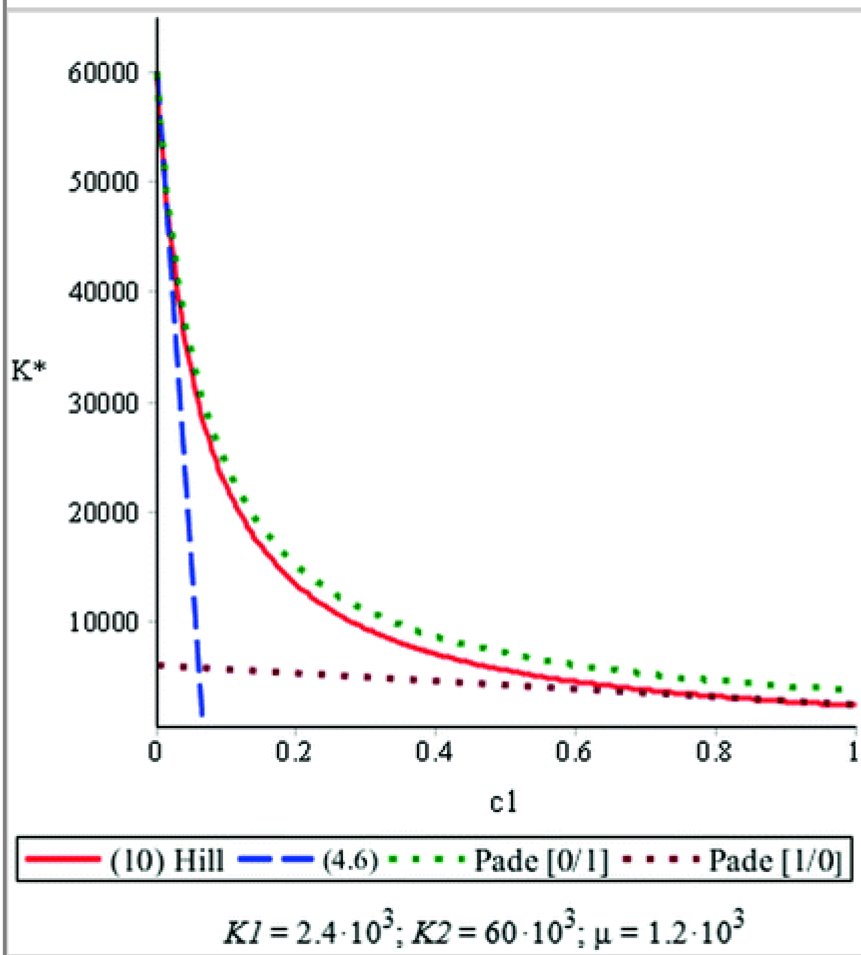
Comparison with the exact solution (10) of expression

$$\mathrm{K}^* = \left[1 + \frac{(3\mathrm{K}_2 + 4\mu)(\mathrm{K}_1 - \mathrm{K}_2)\,\mathrm{c}_1}{(3\mathrm{K}_1 + 4\mu)\,\mathrm{K}_2}\right]\mathrm{K}_2, \tag{11}$$

obtained from (3) in the particular case $\mu_1 = \mu_2 = \mu$, indicates a very limited area of applicability of the latter (Fig. 3, dashed line).

Fig. 3

Comparison of the exact solution (10) with PA (12), (13) in the special case of the same shear modulus of components



Let us transform the solution of (11) to PA [0/1] for a small concentration of inclusions $c_1 \to 0$:

$$K^{*}{}^{(0)}_{[0/1]}(c_1) = \frac{(3K_1 + 4\mu)\,K_2^2}{(3K_1 + 4\mu)\,K_2 - (3K_2 + 4\mu)\,(K_1 - K_2)\,c_1}. \qquad 12$$

Similarly, we construct the PA [1/0] for a large concentration of inclusions $c_2 = 1 - c_1 \to 0$:

$$K^{*}{}^{(1)}_{[1/0]}(c_1) = \frac{(3K_1 + 4\mu)\,K_2 - 3\,(K_1 - K_2)\,K_1 + (3K_1 + 4\mu)\,(K_1 - K_2)\,c_1}{3K_2 + 4\mu}. \qquad 13$$

The PA (12), (13) are close to the exact solution (10) for small and large inclusions, respectively (Fig. 3).

4. Conclusion

The PA (7) reliably describes the effective parameter right up to the beginning of the percolation process and "catches" the percolation threshold.

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