



# Interface model of homogenization for analysing the influence of inclusion size on the elastic properties of composites

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## ABSTRACT

An interface model of homogenization was proposed, this model considers the influence of the inclusions size of the micrometre range on the elastic properties of composites. The appearance of surface strains and shear stresses at the interphase boundary is associated with the "sticking" of the matrix to the surface of the inclusions. The effective modulus of elasticity of a composite is the sum of two terms: a constant part in the form of a modulus of elasticity of a bulk material, and a variable part that is caused by a shift at the interphase boundary and depends on the particles size. Absolute of particles sizes were considered by introducing within the interfacial model empirical elasticity modulus of the composite with the one basic particle size. The results of the calculation are in good agreement with the experimental data for Young's modulus of polymer composites with spherical particles.

## 1. Introduction

The development of new composite materials is closely related to the problem of theoretically forecasting macroscopic or effective properties from the known properties of components and their contents. In the analytical description of the properties of structurally inhomogeneous materials, mean-field theories are commonly used as models of homogenization. The stress and strain fields are statistically averaged, and thus the heterogeneous material is replaced by a homogeneous continuum with a uniform stress–strain state. The main structural factors that affect the properties of composites are the volume fraction, shape, orientation, and particle size. The classical models of homogenization allow us to describe quite accurately the dependences of elastic properties on the content, shape, and orientation of nonspherical particles, but cannot reflect the influence of particle size. At the present time, various interface models are used to describe dimensional effects in micro inhomogeneous materials.

In these interface models, the dependence of the elastic properties of heterogeneous materials on particle size is associated with strains and stresses that are localised at the interphase boundary. Two types of model are used to simulate the properties of the interphase region. In the first type – common boundary or interface models – the discontinuities of displacements and/or stresses are directly connected at the common boundary of the phases; the interphase region is assumed to occupy zero volume. Among the interface models, the linear spring model [1–7] and the interface stress model [6–12] are distinguished.

The second type of model describes the interphase region as an interphase layer that links the particle and the matrix [6,7,13–17]. Moduli of elasticity of the interphase differ from the matrix and particles, and can be homogeneous or variable. Interface models are two-phase models in the sense that the interface region occupies a zero volume fraction. The interphase model is three-phase, consisting of the inhomogeneity, the interphase and the matrix.

As a rule, interface models are used for nanostructured materials. The defining equations of the interface models contain a new non-classical parameter – the internal length  $l_{in}$ , which represents the ratio of the surface elastic constant to the bulk elastic constant [18]. Homogeneous nanostructured materials are characterized by a single surface elastic constant and one internal length. An elastic constant can be found by atomistic modeling. For two-phase composites, the elasticity of an isotropic surface is characterized by two surface elastic constants giving two internal lengths. For heterogeneous materials, atomistic modeling is very difficult and time-consuming [19]. Therefore, atomistic modeling is applicable only to homogeneous nanostructured materials. Since the moduli of elasticity of the interface of heterogeneous materials can not be calculated, they are found from experimental data [20].

The dependence of the elastic properties of nanostructured materials on the dimensions of inhomogeneities is described in the form of scaling laws [7,19,21,22]. The scaling law of elastic properties includes the ratio of the internal length  $l_{in}$  to the characteristic size of the inhomogeneities of  $R$ . For metals and some other materials,  $l_{in}$  usually lies

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within 0.01–0.1 nm and interphase models give a good prediction for inhomogeneities with a size  $R = 3\text{--}5\text{ nm}$  [19]. At sizes of inhomogeneities in excess of 50 nm, the size effect is not described by the interface models [11,19].

To describe the elastic properties with dimensions of inhomogeneities in the micrometre range, interphase layer models are used. Interphase models are various modifications of the three-phase Christensen-Lo model [23]. In contrast to interface models, in the interphase models, classical elastic constants of the interphase are considered. To estimate the effective moduli of elasticity of composites, it is necessary to know the dimensions and elastic moduli of the interphase. Interphases were experimentally found in cement composites and other composite materials [17]. The dimensions of the interphase can be determined directly from the results of microstructural studies. For example, the thickness of the interphase around the aggregate particles in concrete is 10–40  $\mu\text{m}$  [24]. Modules of elasticity of the interphase are adjustable parameters and are determined during the processing of experimental data.

In interphase models, the elastic properties of composites are described within the modified classical models. Under modification the known models are supplemented with new parameters reflecting the properties of the interphase region. Identification of new parameters is performed by the results of experimental studies of the elastic properties of composites with different sizes of particles. The number of dimensions and the laboriousness of the experiment are determined by the number of model parameters.

The interphase layer model was used in Ref. [25]. It was assumed that a strong interphase layer forms on the surface of the spherical particle, which leads to an increase in the effective volume fraction of particles and thus the Young's modulus. On the basis of experimental data, an almost linear dependence of the effective volume fraction on the radius of particles was obtained. To calculate the Young's modulus, a modified Kerner model was used, which includes both the real and effective volume fraction of the particles. To identify the parameters of a linear relationship, experimental data are needed for two sizes of particles. In the model in Ref. [25], there is no physical justification for the linear dependence of the effective volume fraction on the particle radius, and the result can be random. In Ref. [26], a model of the interphase layer was used to describe dimension-dependent elastic properties. The calculated equations contained three adjustable parameters: two characteristic lengths of cohesive phase interactions, and one parameter of adhesion properties of the contacting phases. As a result, it is necessary to have experimental data for three sizes of particles.

In the present work, to describe the effect of the particle size of micrometre scale, an interface model of the common boundary and a physical analogy with the laminar flow of a liquid near a solid wall were considered. In contrast to the known interface models with non-classical elasticity parameters, the proposed model uses the classical elasticity parameters. The calculated dependencies contain one adjustable parameter, and the model is identified by the results of the experiment with one size of the particles.

## 2. Theory and computational dependencies

### 2.1. The model of elastic phase strain at the interphase boundary

Interface models assume discontinuities of displacements and/or stresses at the phase boundary. We will consider two-phase composites with ideal adhesion of the matrix and particles. For ideal adsorption, the displacement field will be continuously along the interface. In this case only tangential surface strains and stresses have non-zero values [27]. Normal components of strains and stresses are considered for jumps of displacements at the interphase boundary [27]. Jumps of displacements appear at break of adhesion bonds and are typical for brittle composites [28,29]. Based on the results of the research

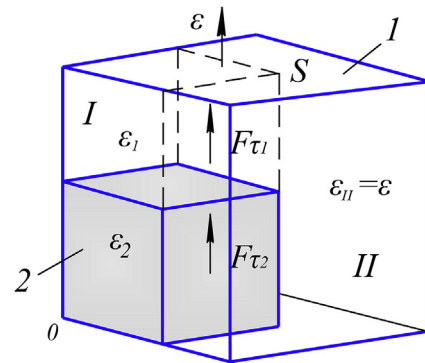


Fig. 1. Takanyagi model for a two-phase isotropic composite.

[27,30,31], only tangential surface strains and stresses of adhesion will be considered. Based on the results of [27,30,31], assuming ideal adhesion, we will only consider tangential surface strains and stresses.

We will consider the effect of surface strains and stresses on the elastic properties of composites on the simplest example of calculating the effective Young's modulus using the Takayanagi model [32]. The representative cell of an isotropic two-phase composite has the shape of a cube with a cubic particle (Fig. 1). A strain  $\epsilon$  of the stretching is specified on the upper cell face.

A representative cell consists of two parallel elements *I* and *II*. The two-phase element *I* is formed by the particle 2 and the fragment of the matrix 1, which are connected in series. The volume of matrix 1 undergoes strain  $\epsilon_1$ . Strain of the volume of particle is  $\epsilon_2$ . The single-phase element *II* is formed only by the matrix 1 and its volume stress is equal to the strain of the cell  $\epsilon$ . The effective Young's modulus of the representative cell will be equal to  $E = \sigma/\epsilon$ , where  $\sigma$  is the stress of the cell. In the classical Takayanagi model, the elements *I* and *II* are deformed independently of each other and the tension of the cell is

$$\sigma_0 = \frac{\sigma_1 S_1 + \sigma_2 S_2}{S}, \quad (1)$$

where  $\sigma_1$  and  $\sigma_2$  are tensile stresses in the volumes of elements *I* and *II*; and  $S_1$  and  $S_2$  are the cross-sectional area of the elements *I* and *II*; and  $S$  is the area of the upper face of the cell.

Let's consider cell deformation under the condition of ideal adhesion of elements *I* and *II*. With ideal adhesion, the strain of the matrix at its vertical boundary with particle will be equal to the strain of the particle  $\epsilon_2$ . At the same time, the strain of the boundary volumes of the matrix is  $\epsilon$ , and  $\epsilon > \epsilon_2$ . As a result, the surface of the matrix at its boundary with particle is under shear strain  $\gamma_{12}$  of magnitude

$$\gamma_{12} = \epsilon - \epsilon_2. \quad (2)$$

The shear stress  $\tau_{12}$  at the vertical boundary of the matrix/particle will be:

$$\tau_{12} = \mu_1 (\epsilon - \epsilon_2), \quad (3)$$

where  $\mu_1$  is the shear modulus of the matrix. Similarly, the vertical surface of the matrix in the element *I* deforms and this surface undergoes a shear strain  $\gamma_{11}$

$$\gamma_{11} = \epsilon_1 - \epsilon. \quad (4)$$

The shear stress  $\tau_{11}$  on the vertical matrix/matrix boundary will be:

$$\tau_{11} = \mu_1 (\epsilon_1 - \epsilon). \quad (5)$$

We perform the summation of the stresses  $\tau_{11}$  and  $\tau_{12}$  over the area and find the shear force  $F_\tau$  on the vertical boundary of the elements:

$$F_\tau = \tau_{11} S_{\tau 1} + \tau_{12} S_{\tau 2}, \quad (6)$$

where  $S_{\tau 1}$  and  $S_{\tau 2}$  are the areas of vertical matrix/matrix boundaries and matrix/particle, respectively. We assign the force  $F_\tau$  to the area of the upper face of the cell and determine the normal stress:

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