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NEAR-SURFACE MASS DEFECT IN MODELS OF LOCALLY HETEROGENEOUS SOLID MECHANICS

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Abstract: This article deals with the model of the locally heterogeneous elastic body. The model accounts for long-range interaction and describes near-surface non-homogeneity and related size effects. The key systems of model equations are presented. From the viewpoint of the representative volume element, the boundary condition for density and the limits of applicability of the model are discussed. The difference of mass density in the near-surface body region from the reference value (near-surface mass defect) causes a non-zero stressed state. It is indicated on the strong dependence of the surface value of density from the curvature of the surface of thin fibres. The effect of the near-surface mass defect on the stressed state and the size effect of surface stresses have been investigated on an example of a hollow cylinder. Size effect of its strength has been studied as well.

Keywords: locally heterogeneous mechanics, RVE, mass defect, size effects, thin fibres

1. INTRODUCTION

In recent decades, various nanoelements are widely used in engineering practice, namely, thin films, fibres and small particles. They are often used to obtain materials and solid bodies with complex microstructure. Such bodies feature comparable surface and volume factors in internal energy.

The basis for studying the behaviour of nanoelements is non-local mathematical models of mechanics, since classical elasticity (e.g., Sneddon and Berry, 1958) that rests upon locality principle fails to describe and predict many observable properties of bodies made of microstructured materials among them surface phenomena and size effect of structural strength. A variety of non-local mathematical models of mechanics is represented in the scientific literature (Eringen, 2002; Karlicic et al., 2015; Khodabakhshi and Reddy, 2015; Matouš et al., 2017). Such models usually take into account long-range interaction, that is, the state at the considered point of the body depends on the state of all points of the body. In peridynamics theory (Silling, 2000), it is done for homogeneous materials by specifying particles force interaction at a finite distance by pairwise force function and considering a peridynamic material without memory, a microelastic material and a structureless material for different simplifying conditions. The models become far more complicated if heterogeneous materials are to be considered.

The models that employ a one-continuum approach to describe the structure of material generally include non-local and gradient models of mechanics. These models are based on a generalisation of the Hooke's law for continuous media. In gradient models, it is done by including spatial derivatives typically of the second order into the relation that links the stress and strain tensors (Aifantis, 2011; Di Paola et al., 2010; Polizzotto, 2003, 2012), or by presenting the dependence between these tensors in the form of spatial functional dependence where the kernel depends on the distance from the point in question to a travelling point (Bažant and Jirásek, 2002; Eringen, 2002; Marotti de Sciarra, 2009). In the last case, it is done by integrating over the region of the body or some neighbourhood of the considered point.

Another approach to describe structural and near-surface non-homogeneities is the local gradient approach in thermomechanics (Burak et al., 2014; Nahirnyj and Tchervinka, 2015, 2018). It is based on the general principles of irreversible thermodynamics and mechanics of rheological systems. Within this approach, a deformable solid is considered as an open thermodynamic system whose mass changes relative to the reference solid. The density and the chemical potential as a conjugated parameter are introduced into the state parameter space. It is efficiently used to describe the structure of material and internal forces in the body. Within models of the approach, the near-surface non-homogeneity of different physical fields and related size effects are caused by the mass defect, that is, the difference of density in the current and reference states. This is consistent with the statement (Silling, 2000) that in a structureless material with no change in the local density of particles, the internal forces are absent.

The parameters in the non-local model are usually associated with the microstructure of the material of the body. The composite materials that are multicomponent systems at microlevel and nanolevel are good examples of microstructured and nanostructured materials; they are widely used in technology due to their advantageous mechanical properties (Wisniewska et al., 2019). These materials are heterogeneous though may consist of essentially homogeneous components. Besides multicomponent materials, there is a variety of structured one-component materials.

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Proper structuring of many ordinary materials may significantly change mechanical, thermal and other physical properties. Bargmann et al. (2018) considering microstructured materials classifies them into non-porous and porous; here one can find an extensive review on investigation methods for the study of heterogeneous materials with respect to geometrical and topological properties of the microstructures. The mechanics and physics of multiphase porous materials at nano and micro scales are considered by Dormieux et al. (2006), Wang and Liew (2007) and others. Cheng (2016) focuses largely on the linear theories, as in the classical linear elasticity and porous medium flow. Note that the mechanical interaction between the solid and the fluid can be very complex while considering one-component material with a variable porosity just one extra parameter may sufficient to analyse the structural influence on averaged material properties.

The study of the material structural influence on solid body properties is the subject of micromechanics. Micromechanics relies on the concept of a representative volume element (RVE) (Bargmann et al., 2018). The RVE-using approaches and techniques in mechanics of heterogeneous media are widely represented in the literature (Drugan and Willis, 1996; Dormieux and Kondo, 2013; Kwok et al., 2015; Guo and Zhao, 2016; Saeb et al., 2016; Bostanabad et al., 2018; Rezakhani et al., 2017; Wisniewska et al., 2019). The RVE is usually regarded as a volume of heterogeneous material that is sufficiently large to be statistically representative of the material (Kanit et al., 2003) or at least large enough to get a sufficiently accurate model to represent mean constitutive response (Drugan and Willis, 1996). The size of the RVE generally depends on the material system as well as the effective property under consideration (Bostanabad et al.,2018; Drugan and Willis, 1996; Kanit et al., 2003; Rezakhani et al., 2017, etc).

The size and shape of RVE can be easily justified for a known periodic structure; however, the majority of microstructures in engineering materials are non-periodic (Bargmann et al., 2018). For random composites, some approaches are presented by Monetto and Drugan (2009), Salmi et al. (2012), Wisniewska et al. (2019) and others. On the other hand, theoretical approaches able to describe structure-related effects in heterogeneous solid bodies (abovementioned non-local and gradient models) do not investigate the RVE-related problem and peculiarities. In these models, the internal scale that is associated with the heterogeneity characteristic size may be used to estimate RVE size.

In this article, we consider the formulation of boundary value problems for bodies with flat and cylindrical boundaries for the local gradient approach. Using RVE formalism, we justify boundary conditions for mass density and discuss the limitation of the model related to parameters of RVE. We also study the influence of surface curvature on near-surface mass defect and size effects for locally heterogeneous bodies.

2. NEAR-SURFACE MASS DEFECT

Thermomechanics of locally heterogeneous solids (local gradient approach in thermomechanics) introduces the energy of structurally heterogeneous material that differs from the energy of classical thermomechanics by term containing a gradient of chemical potential (Burak et al., 2014; Nahirnyj and Tchervinka, 2018). As a consequence, the free energy F for such material depends on the strain tensor e and mass density ϱ. The conjugate parameters are the stress tensor σ and the thermodynamic chemical potential H, respectively. Perturbation of the latter is associated with the binding energy perturbation. The chemical potential is the energy required to change the density per one unit, while other state parameters are constant. It is clear that such energy is different for interior body points and points of the body surface because interior points interact with other body points in their vicinity, while points of the surface interact with the body points not in all directions. Therefore, these parameters (density and chemical potential) allow to describe different interaction conditions in interior and near-surface body regions and thus enable modelling near-surface and structural non-homogeneity. The state parameters space expansion yields mass balance equation modification. The non-homogeneity of the density is the cause of internal forces as well as non-homogeneity of interconnected fields and experimentally observed size effects.

The system of equations for the locally heterogeneous elastic body model, written down for a linearised approach, has the form (Nahirnyj and Tchervinka, 2015):

$$\mu\nabla^2\mathrm{u} + (\lambda+\mu)\nabla(\nabla\cdot\mathrm{u}) - a_m(3\lambda+2\mu)\nabla\varrho = 0,$$
$$\nabla^2\varrho - \xi_m^2(\varrho-\varrho_*) = 0 \qquad (1)$$

if the displacement vector u and mass density ϱ are the key functions and the form

$$\nabla\cdot\sigma = 0,$$
$$\nabla\times\left\{\nabla\times\left[\sigma - \left(\frac{\lambda}{3\lambda+2\mu}\sigma - 2\mu a_m(\varrho-\varrho_*)\right)\mathrm{I}\right]\right\}^T = 0,$$
$$\nabla^2\varrho - \xi_m^2(\varrho-\varrho_*) = 0 \qquad (2)$$

if the stress tensor σ is chosen as a key function instead of displacement u. Here $\sigma = \sigma\colon \mathrm{I}$, I is identity tensor, λ, μ, a_m, ξ_m are constants, ϱ_* is mass density in the reference state, ∇ is del operator, $\cdot, \times, T$ denote inner, vector products and transpose, respectively. The parameter ξ_m^{-1} is a characteristic size of the structural heterogeneity of the material (Nahirnyj and Tchervinka, 2018).

When formulating the boundary value problems, the corresponding boundary conditions need to be supplemented. Generally accepted conditions in the theory of elasticity are the conditions for the stress tensor σ and the displacement vector u in the form:

$$\sigma\cdot n|_{\partial V_\sigma} = \sigma_a, \;\; u|_{\partial V_u} = u_a.$$

Here n is the unit external normal to the body surface ∂V, $(\partial V_\sigma)\cup(\partial V_u) = (\partial V)$.

The analysis of the equation for mass density (second equation of Eq. (1)) shows that its non-trivial solution exists if the value of the body surface mass density ϱ_a differs from the one of the reference body ϱ_*. The question arises what are the reasons and limitations for the surface value of mass density ϱ_a.

For spatially non-local mechanics models, one usually considers the following four states:

- the ideal continuum,
- the heterogeneous continuum,
- the reference body, and
- the actual body within the model.

It should be noted that the equations of non-local theory, in this case the system of Eqs. (1) and (2), are written for a heterogeneous continuum. These equations provide the existence of the RVE in whose region the averaging is carried out. The quanti-

ties and properties describing the behaviour of the body are defined for this element.

For the reference body, we usually take the body of the same configuration as the investigated one without the local heterogeneity and associated effects.

Let us describe in more detail the mass density of the body of structurally heterogeneous material from the viewpoint of RVE. We denote the region of the body by V and the region RVE by Ω. If describing a point deep in the body, then $\Omega \subset V$and the averaged value of the mass density of a structurally heterogeneous body coincides with ones for a structurally heterogeneous media. It is attributed to the RVE centre and is treated as a characteristic of the homogeneous reference body. In the case $\Omega \backslash V \neq \emptyset$, the domain Ω contains the part of the environment and for the mass density holds

$$\varrho = \varrho_* \left(\int_{\Omega \cap V} dV\right)/\left(\int_{\Omega} dV\right), \tag{4}$$

therefore, $\varrho < \varrho_*$.

Let Ω is a sphere of radius R_0 and V is a halfspace (Fig. 1). Moving the RVE from the halfspace depth to its surface, we arrive at mass density value $\varrho_*/2$ when the centre of RVE is at the surface of halfspace. This means that for the flat body boundary, there is a natural boundary condition

$$\varrho|_{\partial V} \equiv \varrho_a = \frac{1}{2}\varrho_*. \tag{5}$$

It may be noted that the real body surface is rough. Thus, the value of the density at the body surface which is described by Eq. (5) must be treated as the upper bound of the surface density of a real body. Postulating constant density in non-local models restricts the characteristic size of the considered body. In this case, the body characteristic size should be much greater than the long-range interaction distance.

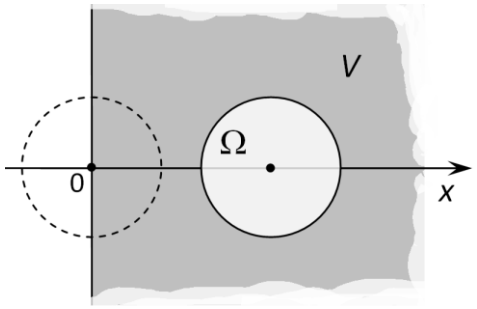

Fig. 1. Spherical representative volume element in the region of halfspaceand at its surface

The mass density in halfspace (region $x \geq 0$) as solution of the problems (1) and (5) has the form:

$$\varrho = \varrho_* - (\varrho_a - \varrho_*)\exp(-\xi_m x). \tag{6}$$

Since ϱ_* is the reference body mass density, the difference $\varrho_* - \varrho$ is the near-surface mass defect in the body actual state.

Based on the analysis of the solution (6), it can be argued that the characteristic size of a representative element (the radius of the sphere R_0) can not be less than $3\xi_m^{-1}$. This restricts the model Eqs. (1) and (2) applicability to flat body boundaries of characteristic size $3\xi_m^{-1}$. The above considerations are also important for models that take into account long-range cohesive forces in the relations for strain and strain tensors and that considers the density to be constant throughout the body.

Sometimes, it is necessary to compare the results for bodies of different geometric configurations, in particular for thin films and fibres as well as for bodies of the same configuration having different characteristic sizes (for instance, fibres of different radii). The question is which mass density value at the cylindrical surface that is equivalent to ones in the boundary condition (5) at the flat surface? Repeating the above arguments for the value ϱ_a^c of mass density at the surface of the cylinder of the radius R_e , we can write:

$$\varrho_a^c = \varrho_* \left\{\frac{1}{2} - \frac{1}{\pi}\int_{\arccos\frac{R_0}{2R_e}}^{\frac{\pi}{2}} \left[1 - 4\left(\frac{R_e}{R_0}\right)^2 \cos^2\varphi\right]^{3/2} d\varphi\right\}. \tag{7}$$

This dependence can be approximated with relative error less than $9.4 \cdot 10^{-4}$ for R_0/R_e in region [0, 0.9] by:

$$\varrho_a^e = \left(0.5 - 0.095\frac{R_0}{R_e}\right)\varrho_*. \tag{8}$$

For mass density at the hollow cylinder inner surface $r = R_i$, we obtain:

$$\varrho_a^i = \left(0.5 + 0.095\frac{R_0}{R_i}\right)\varrho_*. \tag{9}$$

These values tend to the mass density ϱ_a at the surface of the halfspace with radii increase ($R_i \to \infty, R_e \to \infty$) and the surface value of mass density dependence on the radius is more pronounced in thin fibres.

Noteworthy that considered above spherical shape of RVE is one of the most widespread along with cubic shape. If we consider RVE as a cube with edge $2R_1$ and two faces being parallel to the axis of the cylinder, when (7) takes the form:

$$\varrho_a^c = \varrho_* \left\{\frac{1}{2} - \frac{R_e}{2R_1}\left[1 - \frac{\sin^{-1}(R_1/R_e)}{2R_1/R_e} - \frac{1}{2}\sqrt{1 - \left(\frac{R_1}{R_e}\right)^2}\right]\right\}$$

and analogue of (8) is:

$$\varrho_a^e = \left(\frac{1}{2} - \frac{1}{12}\frac{R_1}{R_e} - \frac{1}{80}\left(\frac{R_1}{R_e}\right)^3 + \cdots\right)\varrho_* \approx \left(0.5 - 0.083\frac{R_1}{R_e}\right)\varrho_*.$$

In the case of flat body boundary, the cubic RVE, as well as the spherical RVE, obviously yields $\varrho_a = \varrho_*/2$.

3. STRESSED STATE OF HOLLOW CYLINDER

The body surface curvature effects on the density surface value and the near-surface mass defect, as well as the stress state caused by them, have been studied on the example of the hollow cylinder (region $R_i \leq r \leq R_e$ in the cylindrical coordinates $\{r, \varphi, z\}$). We assume that the cylinder is free of load and at its surfaces $r = R_e$, $r = R_i$, the constant density values are stated according to the formulas (8) and (9).

The distribution of density in the cylinder is described by the formula:

$$\varrho(r) = \varrho_* + \varrho_a^i \frac{K_0(\xi_m R_i)I_0(\xi_m r) - I_0(\xi_m R_i)K_0(\xi_m r)}{I_0(\xi_m R_e)K_0(\xi_m R_i) - I_0(\xi_m R_i)K_0(\xi_m R_e)} +$$

$$+\varrho_a^e \frac{I_0(\xi_m R_e)K_0(\xi_m r) - K_0(\xi_m R_e)I_0(\xi_m r)}{I_0(\xi_m R_e)K_0(\xi_m R_i) - I_0(\xi_m R_i)K_0(\xi_m R_e)},$$

where $I_0(\cdot), K_0(\cdot)$ are the modified Bessel functions of the first and second kinds, respectively.

Fig. 2 shows the density in the cylinder at $R_i/R_e = 0.2; 0.6$ (Fig. 2a and b), $\xi_m R_e = 3,6,12,50$ (curves 1–4).

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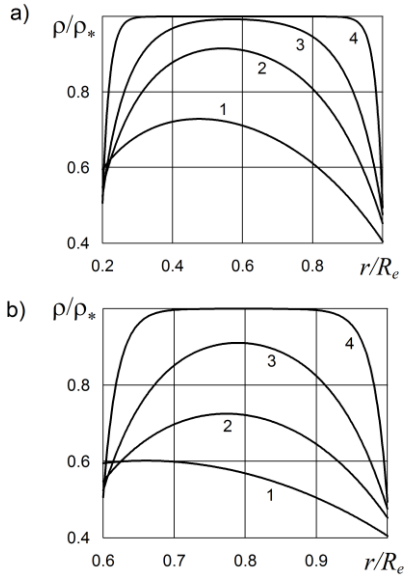

Fig. 2. Distribution of density

If the density ϱ is known, the components $\sigma_{rr}, \sigma_{\varphi\varphi}, \sigma_{zz}$ may be found using the formulae:

$$\sigma_{rr}(r) = a_0 \left[\frac{1}{R_e^2 - R_i^2}\left(1 - \frac{R_i^2}{r^2}\right)\int_{R_i}^{R_e}(\varrho(x) - \varrho_*)x\,dx - \right.$$

$$\left. -\frac{1}{r^2}\int_{R_i}^{r}(\varrho(x) - \varrho_*)x\,dx\right],$$

$$\sigma_{\varphi\varphi}(r) = a_0 \left[\frac{1}{r^2}\int_{R_i}^{r}(\varrho(x) - \varrho_*)x\,dx + \right.$$

$$\left. +\frac{1}{R_e^2 - R_i^2}\left(1 + \frac{R_i^2}{r^2}\right)\int_{R_i}^{R_e}(\varrho(x) - \varrho_*)x\,dx - \varrho(r) + \varrho_*\right], \quad (11)$$

$$\sigma_{zz}(r) = a_0 \left[\frac{2}{R_e^2 - R_i^2}\int_{R_i}^{R_e}(\varrho(x) - \varrho_*)x\,dx - \varrho(r) + \varrho_*\right],$$

where $a_0 = 2\mu a_m\,(3\lambda + 2\mu)/(\lambda + 2\mu)$. The explicit form of the formulae is cumbersome and so it is not presented here.

Figs. 3 and 4 show stresses σ_{rr}/σ_0 and $\sigma_{\varphi\varphi}/\sigma_0 (\sigma_0 = a_0\varrho_*)$, respectively, taking into account (Fig. 3a) and neglecting (Fig. 3b) the dependence of the density surface value on the surface curvature for $\xi_m R_e = 3,6,12,50$ (curves 1–4), $R_i/R_e = 0.2$.

The non-zero stress–strain state in the free body is caused by the mass defect, that is, the difference of the density in the current (actual) state and in the reference one (usually infinite homogeneous media). The distribution and value of stresses are uniquely determined by the characteristics of the material and the geometric characteristics of the body. Comparing Fig 3a and b, we see that taking into account the dependence of the surface value of density on the surface curvature is more significant in thin fibres. Taking into account this dependence can qualitatively change the stress distribution as it is illustrated in particular by the curves 1 in Fig. 3a and b.

Circumferential, $\sigma_{\varphi\varphi}$, and axial, σ_{zz} , stresses are tensile near inner $r = R_i$ and outer $r = R_e$ surfaces of the cylinder and they are compressing in the vicinity of the median surface $r = (R_i + R_e)/2$. Surface stresses $\sigma_{\varphi\varphi}(R_i) = \sigma_{zz}(R_i)$ and $\sigma_{\varphi\varphi}(R_e) = \sigma_{zz}(R_e)$ show size effect. This is exposed in Figs. 5 and 6. Fig. 5 shows the dependence of surface values of stresses $\sigma_{\varphi\varphi}(R_i)/\sigma_0$, $\sigma_{\varphi\varphi}(R_e)/\sigma_0$ (curves 1 and 2) on parameter $\xi_m R_e$ for $R_i/R_e = 0.2$. The dashed line corresponds neglecting the dependence of the density surface value on the surface curvature. Fig. 6 shows the dependence of the values of circumferential stresses at the outer surface of the cylinder $r = R_e$ on parameter R_i/R_e $(R_e - R_i = R_e(1 - R_i/R_e)$ is the thickness of the hollow cylinder wall).

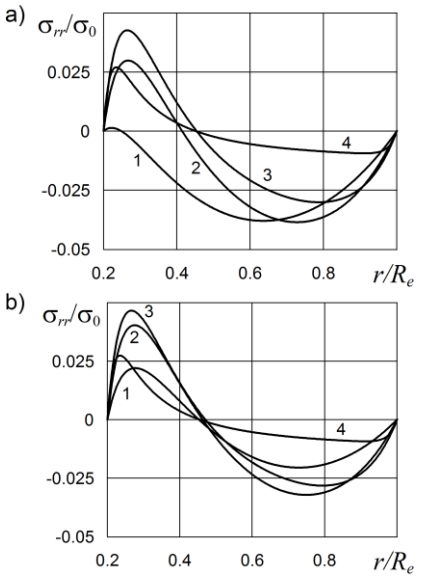

Fig. 3. Distribution of radial stresses

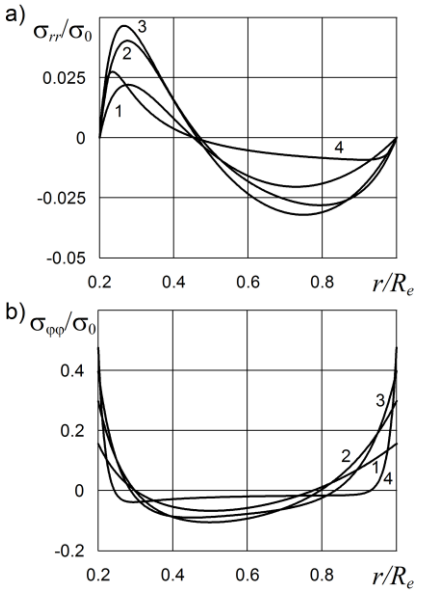

Fig. 4. Distribution of circumferential stresses

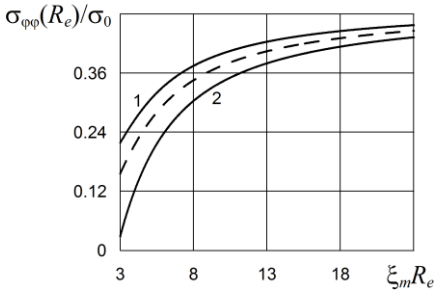

Fig. 5. Size effect of circumferential surface stress

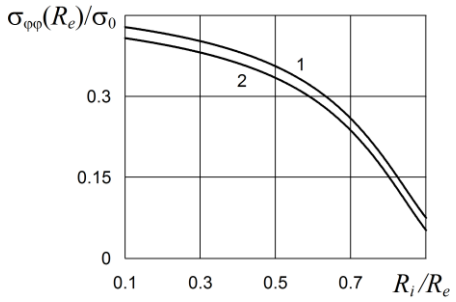

Fig. 6. Circumferential surface stress dependence on R_i/R_e

Taking into account internal stresses is important when calculating operational parameters. Superposing with external force load, they affect the strength characteristics. In the hollow cylinder which is under the action of the force load of intensity σ_a in the direction of the cylinder axis:

$$\int_0^{2\pi}\int_{R_i}^{R_e}\sigma_{zz}(r)r\,dr\,d\varphi = \pi(R_e^2 - R_i^2)\sigma_a$$

the greatest tensile stress is the stress σ_{zz} at the outer cylinder surface $r = R_e$ for which we can write:

$$\sigma_{zz}(R_e) = \sigma_a +$$

$$+a_0\left[\frac{2}{R_e^2-R_i^2}\int_{R_i}^{R_e}(\varrho(x)-\varrho_*)x\,dx - \varrho(R_e) + \varrho_*\right].$$

The method presented by Nahirnyj and Tchervinka (2018) was used to determine the hollow cylinder strength. We assume that the cylinder will fail immediately when the maximum principal stress in at least one point of the body exceeds the tensile strength of the material σ_f. On the basis of Eq. (12) for the load which leads to cylinder fracture, it can be written:

$$\sigma_{cr} = \sigma_+ +$$

$$+a_0\left[\varrho(R_e) - \frac{1}{2}\varrho_* - \frac{2}{R_e^2-R_i^2}\int_{R_i}^{R_e}(\varrho(x)-\varrho_*)x\,dx\right],$$

where:

$$\sigma_+ = \sigma_f - \mu a_m \varrho_* \frac{3\lambda+2\mu}{\lambda+2\mu}$$

is the material parameter which has the meaning of the strength of thick bodies.

Fig. 7 shows the dependence of σ_{cr}/σ_+ on parameter $\xi_m R_e$ (size effect of the strength of the hollow cylinder) for $\sigma_0/\sigma_+ = 16$, $R_i/R_e = 0.2; 0.6$ (curves 1 and 2). The dashed lines correspond to neglecting of the dependence of the density surface value on the surface curvature.

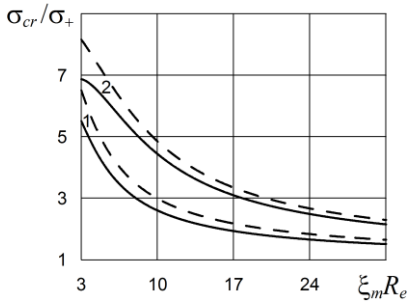

Fig. 7. Size effect of the strength of the hollow cylinder

We see that taking into account the dependence of the surface value of density on the surface curvature is important while calculating the strength of the thin fibres.

4. CONCLUSIONS

The study is concluded to the continual model of mechanics of locally heterogeneous solids which describes near-surface nonhomogeneity and size effects caused by it. The key system consists of equations for stresses (displacements) and the equation for mass density. Formulation of boundary conditions for the mechanical fields and the density is necessary.

A non-zero stress-strained state in a free of external load body in the model is caused by the mass defect, that is, the difference of density in the current and reference states.

The article proposes the method to take properly into account the dependence of the surface value of density on the curvature of the surface. This is important in particular for studying thin fibres. The analysis of the boundary value problems (system of equations and boundary conditions) from the RVE viewpoint allows to determine the limits of applicability of the model as well.

Using the example of the hollow cylinder, it is shown that taking into account the dependence of the surface value of the density on the surface curvature leads to quantitative changes in the values of stresses and also qualitatively change their distribution in thin fibres. This allows correct comparison of stresses in fibres of different radii. (12)

When studying tensile strength of the stretched cylinder within maximum normal stresses theory, the account for the dependence of the surface value of density on the curvature of surface does not change the size effect regularities while reduces the value of the ultimate tensile strength.

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