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Cohesion field: Barenblatt's hypothesis as formal corollary of theory of continuous media with conserved dislocations

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Abstract In the paper the higher-order theory of continuous media with conserved dislocations is developed to describe the spectrum of cohesion and superficial phenomena. A new kinematic interpretation of dislocations is offered, that reflects the connection of dislocations with distortion, with change in volume (porosity), and with twisting. The main aim of the paper is to receive the strong theoretical justification for famous hypothesis of Barenblatt about cohesion field near top of crack. A new variants of the fracture criterions are discussed that based on the of the theory of media with microstructures, connection of the length of the cohesion interaction zone (a new physical constant) with parameters of the fracture mechanics is established.

Keywords Multiscale modeling · Cohesion field · Adhesion · Fracture

1 Introduction

In present research work the higher-order theory of continuous media with conserved dislocations is developed to describe the spectrum of cohesion and superficial phenomena. The special attention is paid to the analysis of kinematic relations since in the framework of variational description the kinematics of medium fully defines the system of internal volumetric and surface interactions of the body under study. The correct consistent theory of continuous media is constructed using the variant of the kinematics variation principle. The sequential description of kinematics of media with possible internal structures (field of defects) of the various scales is introduced, to investigate defective media with kept defects-dislocations, to describe of the defects generation conditions. This approach allows introducing the set of internal interactions of various types consequently, which correspond to various types of microstructures in the considered media. The formulation of governing equations

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(fundamentals) and the statement of boundary conditions for multi-scale modeling of the material are given.

The presented generalized continuum mechanics model is a theoretical model in which the surface traction, the meniscus, wettability and capillarity are modeled as particular the scale effects within the framework of the unified continual description. On the basis of the carried out kinematic analysis a novel classification of dislocations is offered (see Lurie and Belov 2005, 2006). Applied closed theory of the media with microstructure is proposed, which allow to receive the strong theoretical justification for famous hypothesis of Barenblatt (see Barenblatt 1961/1962). As a result the nonsingular stresses are modelled in top of a crack (nonclassical effect). It is established on connection of length of the cohesion interaction zone (a new physical constant) with parameters of the fracture mechanics.

The variant of criterion of fracture, which is the criterion of the macro-crack appearance is proposed. The criterion of the crack development is offered with using of density of superficial energy. Using the nonclassical asymptotic solution the variant of the Hall-Petch formula for different scales is established (see also Gutkin and Ovidko 2003).

2 Basics of the theory of continuous media with conserved dislocations

In present research work the higher-order theory of continuous media with conserved dislocations is developed to describe the spectrum of cohesion and superficial phenomena. Let's present shortly the kinematical basics of the theory, constitutive equations, mathematical variational formulation of the theory and some previously results. The kinematic model of this theory defines by the non-symmetric Cauchy relations and Papkovich non-homogeneous equations (see Belov and Lurie 2006):

$$d^0_{in} = R_{i,n}, \quad \text{and} \quad d_{in,m} \ni_{nmj} = \Xi_{ij} \tag{1}$$

here $d_{in} = \gamma_{in} + (1/3)\theta\delta_{in} - \omega_k \ni_{ink}$, R_i is the continuous displacement vector, d^0_{ij} is the distortion tensor, γ_{in} is a strain deviator tensor, θ—change in volume, ω_k—vector of elastic spins (a pseudovector), $\ni_{ijk}$ is the permutation symbol, δ_{ij} is the Kronecker delta, Ξ_{ij} is a second-rank pseudotensor and defines an incompatibility of displacements of displacements (De Wit 1960).

The Papkovich homogeneous equations $d_{in,m} \ni_{nmj} = 0$ can be interpreted as the existence condition for the vector potential R_i, then the displacement vector R_i is a vector potential for the distortion tensor d^0_{ij}. The solution of the Papkovich non-homogeneous equations can be represented as the following sum: $d_{ij} = d^0_{ij} + d^{\Xi}_{ij} = R_{i,j} + d^{\Xi}_{ij}$, where d^0_{ij} is the solution of the Papkovich homogeneous equation ($d^0_{ij} = R_{i,j}$) and d^{Ξ}_{ij} is a partial solution of the Papkovich non-homogeneous equation. No continuous vector potential exists for the partial solution of the Papkovich non-homogeneous equations, and only the following representation can be written for it: $d^{\Xi}_{in} = \gamma^{\Xi}_{in} + (1/3)\theta^{\Xi}\delta_{in} - \omega^{\Xi}_k \ni_{ink}$. Along with continuous d^{Ξ}_{ij} one can consider as the generalized displacements the following quantities: γ^{Ξ}_{ij}, ω^{Ξ}_k and θ^{Ξ}. So, definitions of tensors of free distortion, d^{Ξ}_{ij}, and constrained distortion, d^0_{ij} are introduced. The defective displacement field represents the superposition of two fields: R_i and $\int_{M_0}^{M_x}[\gamma^{\Xi}_{ij} + (1/3)\theta^{\Xi}\delta_{ij} - \omega^{\Xi}_k \ni_{ijk}]dy_j$; $(R_i + \int_{M_0}^{M_x}[\gamma^{\Xi}_{ij} + (1/3)\theta^{\Xi}\delta_{ij} - \omega^{\Xi}_k \ni_{ijk}]dy_j)$. However, unlike of the Cesaro formulae, the above integrand does not satisfy the integrability conditions $[\gamma^{\Xi}_{in} + (1/3)\theta^{\Xi}\delta_{in} - \omega^{\Xi}_k \ni_{ink}]_{,m} \ni_{nmj} = d^{\Xi}_{in,m} \ni_{nmj} = \Xi_{ij} \neq 0$.

Three types of dislocations are defined, namely related to γ_{ij}^{Ξ}, ω_k^{Ξ} and θ^{Ξ}: $\Xi_{ij} = [\gamma_{in}^{\Xi} + (1/3)\theta^{\Xi}\delta_{in} - \omega_k^{\Xi}\,\ni_{ink}]_{,m}\,\ni_{nmj} = (\Xi_{ij})_\gamma + (\Xi_{ij})_\theta + (\Xi_{ij})_\omega$. The quantities $(\Xi_{ij})_\gamma$, $(\Xi_{ij})_\theta$, and $(\Xi_{ij})_\omega$ are the sources of the corresponding three types of dislocations: γ—dislocations, θ–dislocations and ω–dislocations. The law of conservation of dislocations has place:

$$\Xi_{ij,j} = 0$$

The integral analogue of the law of conservation of dislocations can be written as follows:

$$\iiint \Xi_{ij,j}\,dV = \oint\!\!\oint \Xi_{ij}n_j\,dF = 0.$$

The sources of the corresponding three types of dislocations $(\Xi_{ij})_\gamma$, $(\Xi_{ij})_\theta$ and $(\Xi_{ij})_\omega$ are satisfied by the conservation laws separately:

$$[(\Xi_{ij})_\gamma]_{,j} = 0, \quad [(\Xi_{ij})_\theta]_{,j} = 0, \; [(\Xi_{ij})_\omega]_{,j} = 0.$$

As a measure of defectiveness (dislocations) one can choose a flux of tensor Ξ_{ij} through the plane of the chosen flat integration contour: $\iint_F \Xi_{ij}n_j\,dF = n_j \iint_0 \Xi_{ij}\,dF$.

Let' consider the plane contour where s_j is a unit vector tangential to the plane contour of integration; n_n is a constant normal vector to the plane of contour of integration; and vectors s_j, v_m, n_n form the vector basis at the current point of the contour. Then a Burgers vector is introduced:

$$b_i = \oint d_{ij}^{\Xi}dx_j = \oint d_{ij}^{\Xi}s_j\,ds,$$

or

$$b_i = \oint d_{ij}^{\Xi}v_m n_n \ni_{jmn}ds = \iint \Xi_{in}n_n\,dF = n_n \iint \Xi_{in}\,dF.$$

Three type of a Burgers vector $(b_i)_\gamma$, $(b_i)_\theta$, $(b_i)_\omega$ is introduced using suggested classification of three type of dislocation:

$$b_i = \oint \gamma_{ij}^{\Xi}s_j\,ds + \frac{1}{3}\oint \theta^{\Xi}s_i\,ds - \oint \omega_k^{\Xi}\ni_{ijk}s_j\,ds = (b_i)_\gamma + (b_i)_\theta + (b_i)_\omega \tag{2}$$

We call $(b_i)_\gamma$ as the dislocation the of quantity γ_{ij}^{Ξ}; $(b_i)_\theta$ as the dislocation of quantity θ^{Ξ}; and consequently, $(b_i)_\omega$ as the dislocation of ω_k^{Ξ}.

In the works Lurie and Belov (2005, 2006) the kinematical variation method of modeling is formulated. The virtual work of internal forces is postulated as a virtual action of reaction force factors on the kinematical connections (1) peculiar to the medium. This equation is presented as a linear form of variations of its arguments and can be integrated for the conservative mediums.

$$U = \iiint_V U_V\,dV + \oint\!\!\oint_F U_F\,dF, \quad U_V = U_V(d_{ij}^0; d_{ij}^{\Xi}; \Xi_{ij}), \quad U_F = U_F(d_{ij}^{\Xi}) \tag{3}$$

Stating physical linearity of the model, the density of potential energy U of the model in (3) can be found in a bilinear quadratic form of its own arguments of the different tensor's dimensions:

$$2U_V = 2U_V(d_{ij}^0; d_{ij}^{\Xi}; \Xi_{ij}) = 2U_V(s_{ij}^{\alpha}) = c_{ijnm}^{\alpha\beta}s_{ij}^{\alpha}s_{nm}^{\beta} \tag{4}$$

where Greek indexes α ($\alpha = 1, 2, 3$) denote the space of generalized kinematic variables $s_{ij}^1 = d_{ij}^0$, $s_{ij}^2 = d_{ij}^{\Xi}$, $s_{ij}^3 = \Xi_{ij}$; $c_{ijnm}^{\alpha\beta}$ is the tensors of elastic coefficients.

For isotropic, nonsymmetrical model of bodies $c_{ijnm}^{\alpha\beta}$ is in (4) the isotropic tensors of fourth rank, constructed as a product of the pairs of Kronecker's tensors with all possible permutations of indexes, $c_{ijnm}^{\alpha\beta} = c_1^{\alpha\beta}\delta_{ij}\delta_{nm} + c_2^{\alpha\beta}\delta_{in}\delta_{jm} + c_3^{\alpha\beta}\delta_{im}\delta_{jn}$, (for symmetrical model $c_2^{\alpha\beta} = c_3^{\alpha\beta}$):

$$\begin{aligned}2U_V &= \left(c_2^{\alpha\beta} + c_3^{\alpha\beta}\right)\gamma_{nm}^{\alpha}\gamma_{nm}^{\beta} + (1/3)\left(3c_1^{\alpha\beta} + c_2^{\alpha\beta} + c_3^{\alpha\beta}\right)\theta^{\alpha}\theta^{\beta} + \left(c_2^{\alpha\beta} - c_3^{\alpha\beta}\right)\omega_{nm}^{\alpha}\omega_{nm}^{\beta} \\ &= 2\mu^{\alpha\beta}\gamma_{nm}^{\alpha}\gamma_{nm}^{\beta} + (1/3)(2\mu^{\alpha\beta} + 3\lambda^{\alpha\beta})\theta^{\alpha}\theta^{\beta} + 2\chi^{\alpha\beta}\omega_{nm}^{\alpha}\omega_{nm}^{\beta} \qquad (5)\end{aligned}$$

$\mu^{\alpha\beta}$ are the analogs of the shear moduli; $2\mu^{\alpha\beta} + 3\lambda^{\alpha\beta}$ are defined the spherical tensors; $\chi^{\alpha\beta}$ are the third Lame coefficients for nonsymmetrical model.

Density of the adhesion energy on the body surface can be expressed as follows:

$$2U_F = A_{ijnm}d_{nm}^{\Xi}d_{ij}^{\Xi} \qquad (6)$$

The energy of adhesion (6) is defined not from all the nine components of the tensor of free distortion d_{in}^{Ξ}, but only from six of them $d_{im}^{\Xi}(\delta_{pm} - n_p n_m)$ in the model of media with conserved dislocation. So, the complete variationl correct model of media with the conserved dislocations is as a result formulated:

$$\begin{aligned}L = A-(1/2)\iiint\left\{c_{ijnm}^{11}R_{n,m}R_{i,j} + 2c_{ijnm}^{12}R_{n,m}d_{ij}^{\Xi} + c_{ijnm}^{22}d_{nm}^{\Xi}d_{ij}^{\Xi} + c_{ijnm}^{33}\Xi_{nm}\Xi_{ij}\right\}dV \\ -(1/2)\oiint\left[\left(\delta_{mp} - n_m n_p\right)\left(\delta_{jk} - n_j n_k\right)A_{ijnm}d_{nm}^{\Xi}d_{ij}^{\Xi}\right]dF \qquad (7)\end{aligned}$$

The constants in the bilinear quadratic form in Eq. 7 are, therefore, physical constants of the model and thus establish a generalized equation of the Hook's law in the volume and on the surface (constitutive relations):

$$\begin{aligned}&\sigma_{ij} = c_{ijnm}^{11}R_{n,m} + c_{ijnm}^{12}d_{nm}^{\Xi}, \quad p_{ij} = c_{ijnm}^{21}R_{n,m} + c_{ijnm}^{22}d_{nm}^{\Xi}, \quad m_{ij} = c_{ijnm}^{33}\Xi_{nm}, \\ &M_{ij} = A_{ijnm}d_{np}^{\Xi}\left(\delta_{mp} - n_m n_p\right) \qquad (8)\end{aligned}$$

here σ_{ij} are stresses, m_{ij} are moment stresses in the volume, p_{ij} are dislocation stresses, M_{ij} are moment stresses on the surface.

Equations 7, 8 give the mathematical formulation of the theory for the media with conserved dislocations.

Tensor of modulus of elasticity with indexes "11" in Eqs. 5, 7, 8 defines the mechanical properties of media that is not damaged by the dislocations; tensor of modulus with indexes "22" is damaged by the dislocations; tensor of modulus with indexes "12" defines the mutual disturbance of a classical displacement field and purely dislocation states.

In the case if $c_{ijnm}^{12} \neq 0$, the mutual disturbance of a classical displacement field and purely dislocation states occurs. The cross-linked terms in the Hooke's law for σ_{ij} and p_{ij} reflect these disturbances.

The part of the strain energy density related to the dislocation tensor $c_{ijnm}^{33}\Xi_{ij}\Xi_{nm}$ defines the rapidly varying local part of the potential energy of dislocations. The remaining part of the strain energy density is slow varying, and it can be represented as a sum of potential energies of following three types of dislocations: γ—dislocations, θ—dislocations and ω—dislocations. Hence, the slow varying part of the strain energy does not contain any cross-linked terms of the above-indicated types of dislocations, and it is the additive form for the components of free distortion. Therefore, for the approximate estimates in this kind of problems, one may neglect the local rapidly varying part of energy. Herewith, the additivity in decomposition of the potential energy density into the components of free distortion takes place indeed.

The potential energies of free distortion, change of volume, and torsion, do not have any cross-linked terms. So, the potential energies of the introduced types of dislocations can be added to each other, and they can exist isolated and independent of other sorts of dislocations.

The proposed classification makes it possible to predict special cases of media with the conserved dislocations, when in continuous medium prevails only one or two types of dislocations. In fact, the offered classification allows prediction of certain particular cases of dislocations when only one or two types of dislocations are dominating in the medium. We can do it introducing different definitions for free distortion tensor d_{ij}^{Ξ}. For example, in the medium with distributed curls the only dominating dislocations are those generated by the free rotational deformations ω_k^{Ξ}. A "classical" type of the Cosserat media model for which $\gamma_{ij}^{\Xi} = 0$ and $\theta^{\Xi} = 0$, and the free distortion tensor is determined by a relation $d_{ij}^{\Xi} = -\omega_k^{\Xi} \ni_{ijk}$, can be obtained as a particular case of the general model. Analogously, the porous medium also can be considered as a particular case of the general model. In the porous medium the only dominating dislocations are those generated by free volume change θ^{Ξ}. Therefore, for the porous medium with four degrees of freedom R_i, θ^{Ξ}, we get $\omega_k^{\Xi} = 0$, $\gamma_{ij}^{\Xi} = 0$ and $d_{ij}^{\Xi} = (1/3)\theta^{\Xi}\delta_{ij}$. In such particular models it is possible to reduce a number of degrees of freedom, which substantially facilitates the analysis of the separate properties of media with the conserved dislocations.

Note that the wide set of the particular applied theory of media in the displacements with six boundary conditions at each regular point of body surface can be received using generalized Aero-Kuvshinskii's hypothesis about the proportionality of free distortion tensor and some linear combination of components of restricted deformations:

$$d_{ij}^{\Xi} = aR_{k,k}\delta_{ij} + bR_{i,j} + cR_{j,i} = a_{ijpq}R_{p,q}, \qquad (9)$$
$$\text{where } a_{ijpq} = a\delta_{ij}\delta_{pq} + (b+c)\delta_{ip}\delta_{jq} + (b-c)\delta_{iq}\delta_{jp}$$

The different particular models can be established by means of choosing parameters a, b, c in Eqs. 9.

3 Surface basics of the theory of continuous media with conserved dislocations

The surface potential energy will have a form of a quadratic function of only six "plane" components of free distortion $d_{ik}^{\Xi}(\delta_{jk} - n_j n_k)$ and the adhesion modulus tensor. Structure of the adhesion modulus tensor, A_{ijnm}, is determined by its decomposition into the fourth rank tensors constructed as all possible products of pairs of "plane" Kronecker's tensors and the tensors formed as products of unit normal vectors of $n_i n_j$ type, with all the possible permutations of indexes. In addition to that, we will take into account that the potential energy of adhesion should not depend on the components of the free distortion tensor having a last index equal to the index of the unit normal vector to the surface. As a result, the adhesion modules tensor can be represented as follows (see Lurie and Belov 2005, 2006):

$$\begin{aligned} A_{ijnm} = \Big[& \lambda^F (\delta_{ij} - n_i n_j)(\delta_{nm} - n_n n_m) + \eta^F n_i n_n (\delta_{jm} - n_j n_m) \\ & + \left(\mu^F + \chi^F\right)(\delta_{in} - n_i n_n)(\delta_{jm} - n_j n_m) + \left(\mu^F - \chi^F\right) \\ & \times (\delta_{im} - n_i n_m)(\delta_{jn} - n_j n_n)\Big] \end{aligned} \qquad (10)$$

where λ^F is an adhesion analogue of the Lame coefficient, μ^F is the adhesion analogue of the shear modulus, χ^F is an adhesion analogue of the second Lame coefficient in non symmetric theory of elasticity, η^F is an adhesion analogue of the Winkler rigidity of an "internal underlayer" of the surface producing the reaction moment proportional to the free rotations of the midline of the surface (the near-surface layer) in two orthogonal directions.

It can be shown (see Lurie and Belov 2005, 2006) that this adhesion modulus are described the effect of the surface tension; effects of the distortion and torsion in the plane tangent to the surface correspondingly, that are modeled friction of two half-spaces with ideally smooth contact surface; and at last, the effect of surface bending, that represents the deformation of the "inner Winkler springs".

4 Modeling of the cohesion field

Let's consider the gradient, applied theory on the base of the generalized Aero-Kuvshinskii's hypothesis (9). Using (11) we can find the pseudotensor of dislocation Ξ_{ij}: $(R_{i,nm}\,\ni_{nmj} = 0)$

$$\begin{aligned}\Xi_{ij} &= d^{\Xi}_{in,m}\,\ni_{nmj} = aR_{k,km}\,\ni_{imj} + (b-c)R_{n,im}\,\ni_{nmj}\\ &= -\left[a\theta^0{}_{,m}\,\ni_{ijm} + 2(b-c)\omega^0_{j,i}\right]\end{aligned} \tag{11}$$

The Lagrangian and variation formulation for generalized Aero-Kuvshinskii's model respect to displacement vector only can be written with the aid of Eqs. 11:

$$\begin{aligned}L = A - (1/2)\iiint &\Big\{C_{ijnm}R_{n,m}R_{i,j} + 4a^2\chi^{33}\theta^0{}_{,k}\theta^0{}_{,k} + 4(b-c)^2(\mu^{33}+\chi^{33})\omega^0_{i,j}\omega^0_{i,j}\\ &+ 8a(b-c)\chi^{33}\theta^0{}_{,k}\,\omega^0_{i,j}\,\ni_{ijk} + 4(b-c)^2(\mu^{33}-\chi^{33})\omega^0_{i,j}\omega^0_{i,j}\Big\}\,dV\\ &-(1/2)\oint\!\!\!\oint A_{ijnm}R_{n,m}R_{i,j}\,dF\end{aligned} \tag{12}$$

here C_{ijnm} and A_{ijnm} are generalized damaged moluli of elasticity in the volume and on the surface, that can be written as

$$\begin{aligned}C_{rspq} &= c^{11}_{rspq} - 2(c^{12}_{ijrs}\,a_{ijpq}) + (c^{22}_{ijnm}\,a_{nmrs}\,a_{ijpq})\\ &= \lambda\delta_{rs}\delta_{pq} + (\mu+\chi)\delta_{rp}\delta_{sq} + (\mu-\chi)\delta_{rq}\delta_{sp},\end{aligned} \tag{13}$$

$$\begin{aligned}\lambda &= (2\mu^{11}/3 + \lambda^{11}) - 2(3a+2b)(2\mu^{12}/3 + \lambda^{12}) + (3a+2b)^2(2\mu^{22}/3 + \lambda^{22})\\ &\quad -(2/3[\mu^{11} - 4b\mu^{12} + 4b^2\mu^{22}],\\ \mu &= \mu^{11} - 4b\mu^{12} + 4b^2\mu^{22}, \qquad \chi = \chi^{11} - 4c\chi^{12} + 4c^2\chi^{22}\end{aligned}$$

and

$$\begin{aligned}A_{ijnm} = {}&[4(a+b)^2(\lambda^F + \mu^F) - 4b^2\mu^F](\delta_{ij} - n_in_j)(\delta_{nm} - n_nn_m)\\ &+ (b+c)^2\delta^F n_in_n(\delta_{jm} - n_jn_m)\\ &+ 4(b^2\mu^F + c^2\chi^F)(\delta_{in} - n_in_n)(\delta_{jm} - n_jn_m) + 4(b^2\mu^F - c^2\chi^F)\\ &\quad\times(\delta_{im} - n_in_m)(\delta_{jn} - n_jn_n)]\\ &+ 4(3a+2b)^2(\lambda^F + \mu^F)n_in_nn_jn_m + (b-c)^2\delta^F(\delta_{in} - n_in_n)n_jn_m\end{aligned} \tag{14}$$

Note that μ^F, λ^F, χ^F and δ^F are the damaged adhesion modulus. As particular case the more simplified adhesion model (Lurie et al. 2006) can be received from Eqs. 14. Assume that $\mu^F = \chi^F = 0$, and $a = -b = c$. Then we can find the following equations for adhesion modulus:

$$A_{ijnm} = D_{in}n_j n_m = An_i n_n n_j n_m + B(\delta_{in} - n_i n_n)n_j n_m$$
$$= 4a^2\lambda^F n_i n_n n_j n_m + 4a^2\delta^F(\delta_{in} - n_i n_n)n_j n_m$$

In the last equation constants A and B have the clear physical sense. The coefficient B is responsible for the surface effects at each point of the surface within the tangential plane; the coefficient A is responsible for the adhesion interaction normal to the surface.

The equations of the Hook's law in the volume and on the surface (constitutive relations) can be easy established:

$$\sigma_{ij} = \partial U_V/\partial R_{i,j}, \quad a_{ij} = \partial U_F/\partial R_{i,j},$$
$$m_{ij} = \partial U_V/\partial \omega^0_{i,j}, \quad m_k = \partial U_V/\partial(\theta^0{}_{,k}). \tag{15}$$

Here σ_{ij} and a_{ij} are stresses in the volume and adhesion stresses on the surface, m_{ij} is the moment stresses and m_k is the vector of forces associated with porous dislocations

The Eqs. 11–15 are defined the closed generalized of Aero-Kuvshinskii's model.

The following theorems have place.

Theorem 1 *1. For arbitrary vector field φ_i the following variation formulation of the Aero-Kuvshinskii's model has place (for smooth contour):*

$$\delta L = \iiint \left\{ \frac{\partial \tau_{ij}}{\partial x_j} + P_i^V \right\} \delta R_i dV$$
$$+ \oiint \left\{ \left[P_i^F - \tau_{ij} n_j + (\delta_{pj} - n_p n_j)\frac{\partial b_{ij}}{\partial x_p} \right] \delta R_i - b_{ij} n_j \delta \dot{R}_i \right\} dF = 0, \tag{16}$$

$$\tau_{ij} = \sigma_{ij} - m_{k,k}\delta_{ij} + (1/2)m_{kq,q}\,\Im_{ijk} - 2\mu(\varphi_{k,k}\delta_{ij} - \varphi_{j,i}),$$
$$b_{ij} = a_{ij} + m_k n_k \delta_{ij} - (1/2)m_{kq}n_q\,\Im_{ijk} + 2\mu\varphi_p n_q \Im_{ipr}\Im_{jqr}. \tag{17}$$

2. *Equilibrium equations in (16) have a classical view for tensor τ_{ij}, which we will call as "classical" tensor of stresses.*
3. *Additional force vector $B_i = (\delta_{pj} - n_p n_j)b_{ij,p}$ defines non-classical effects in the boundary conditions, B_i is the plane divergence of tensor b_{ij}, which we will call as tensor of Barenblatt's stresses. In Eq. 16, P_i^V and P_i^F are vectors of given densities of loads in the volume V and on the surface F.*

Theorem 2 *1. Equilibrium equations of generalized Aero-Kuvshinskii's model in displacement can be written in the following alternative forms:*

(a) $L_{ij}(\cdot)\{R_j - g_1[\partial^2 R_k/\partial x_j\partial x_k] - g_2[\Delta(R_i) - \partial^2 R_k/\partial x_j \partial x_k]\} + P_i^V = 0$
(b) $\{(\cdot)\delta_{ij} - g_1[\partial^2(\cdot)/\partial x_j \partial x_i] - g_2[\Delta(\cdot)\delta_{ij} - \partial^2(\cdot)/\partial x_j\partial x_i]\} L_{jk}R_k + P_i^V = 0$ *where* $L(\cdot) \equiv L_{ij}(\cdot) = (2\mu+\lambda)\partial^2(\cdot)/\partial x_j\partial x_i + (\mu+\chi)(\Delta(\cdot)\delta_{ij} - \partial^2(\cdot)/\partial x_j \partial x_i)$ *is a classical Lame operator,* $g_1 = 4a^2\chi^{33}/(2\mu+\lambda)$, $g_2 = (b-c)^2(\mu^{33}+\chi^{33})/(\mu+\chi)$

2. *The following two form solutions of the equilibrium equations can be proposed:*

(a) $U_i = R_i - g_1\partial^2(R_j)/\partial x_j \partial x_i - g_2[\Delta(R_i) - \partial^2(R_j)/\partial x_j\partial x_i]$ *and* $L_{ij}(U_j) + P_i^V = 0$ *or* $L(\vec{U}) + \vec{P}^V = 0$, *here* $L(\vec{U}) \equiv L_{ij}(U_j)$ *Vector function* U_j *is satisfied of the*

classical equilibrium equations and we will call one as "classical" displacement vector

(b) $u_j = -(1/C)L(\vec{R}) \equiv -(1/C)L_{jk}(R_k)$ and $M^C(\vec{u}) \equiv M^C_{ij}(u_j) + P^V_i = 0$, $M^C(\vec{u}) \equiv M^C_{ij}(u_j)$, where C is some constant; $M^C(\cdot) \equiv M^C_{ij}(\cdot) \equiv \tilde{g}_1[\partial^2(\cdot)/\partial x_j \partial x_i] + \tilde{g}_2[\delta_{ij}\Delta(\cdot) - \partial^2(\cdot)/\partial x_j \partial x_i] - C\delta_{ij}(\cdot)$, $\tilde{g}_1 = Cg_1$, $\tilde{g}_2 = Cg_2$ Vector-function $\vec{u} = u_j$ satisfies of the non-classical Helmgoltz type equations in which constant C is some physical constant that determine the local interactions; we will call u_j as "Cohesion" displacement vector.

3. Any solution of the equation $LM^C(\vec{R}) = 0$, can be submitted as $\vec{R} = \vec{U} - \vec{u}$, где $L(\vec{U}) = 0$, $M^C(\vec{u}) = 0$. Indeed $LM^C(\vec{R}) = M^C L(\vec{U}) - LM^C(\vec{u}) = 0$
4. Assume that $C = (2\mu + \lambda)^2/4a^2\chi^{33} = (\mu + \chi)^2/(b - c)^2(\mu^{33} + \chi^{33})$. Then

(a) physical constants μ^{33} and χ^{33} can be found from constant C:

$$\mu^{33} = (1/C)[(\mu + \chi)^2/(b - c)^2 - (2\mu + \lambda)^2/4a^2],$$
$$\chi^{33} = (1/C)(2\mu + \lambda)^2/4a^2$$

(b) the following relations are

$$M^C(\cdot) \equiv L^C(\cdot), \text{ and } \vec{U} = -(1/C)L^C(R_i) \text{ or } U_j = (1/C)[\delta_{ij}(R_i) - (1/C)L_{ij}(R_i)]$$

(c) the following expansion has place: $\vec{R} = \vec{U} - \vec{u}$.

It can be easy proof: $\vec{U} = -(1/C)L^C(R_i) = \vec{R} - (1/C)L(\vec{R}) = \vec{R} + \vec{u}$

Theorem 3 *If $\mu^{33} = 0$, then:*

1. The following simplified multiscale model of the cohesion field is formulated:

$$L = A - (1/2)\iiint \{C_{ijnm}R_{n,m}R_{i,j} + Cu_iu_i\}\,dV - (1/2)\oiint A_{ijnm}R_{n,m}\,R_{i,j}\,dF \tag{18}$$

where $\vec{u} = -(1/C)L(\vec{R})$, or $u_i = -(1/C)L_{ij}(R_j)$
2. The following consequence results from Theorem 1 and Theorem 2.

Classical stresses in Eqs. 16, 17 can be written only from classical displacement vector U_i, if we will put $\varphi_k = u_k$ in Eqs. 17:

$$\tau_{ij} = \lambda U_{k,k}\delta_{ij} + \mu(U_{i,j} + U_{j,i})$$

Full stresses $\sigma_{ij} = C_{ijnm}R_{n,m}$ is linear combination from classical stresses τ_{ij} and Cohesion stresses $t_{ij} = C_{ijnm}u_{n,m}$; $\sigma_{ij} = \tau_{ij} - t_{ij}$

Cohesion stresses are defined by the following equilibrium equation

$$t_{ij,j} - Cu_i + P^V_i = 0.$$

Proposed multi scale model describes simultaneously the classical stress- strain state (defines by the stress and deformations tensors τ_{ij}, $U_{i,j}$) and cohesion stress-strain state with tensor of cohesion stresses t_{ij}, and with field of Cohesion deformation $u_{n,m}$.

5 Nonsingular cracks

Assume that adhesion physical constants in Eq. 18 are zero, in other words the adhesion properties are ignored. The following question is interesting. There are exist the formulations of the boundary problems when the common problem can be divided into the unrelated boundary problems for classical displacements U_i and for cohesion displacements u_i problems separately?

Let's consider the variation boundary problem (18) for isotropic material and use the expansion $\vec{R} = \vec{U} - \vec{u}$:

$$L = A(U) - A(u) - (1/2) \iiint_V \left[\sigma_{ij}^U \varepsilon_{ij}^U + \sigma_{ij}^u \varepsilon_{ij}^u - 2C_{ijnm} \varepsilon_{ij}^U \varepsilon_{ij}^u + C u_i u_i \right] dV$$

$$= L(U) + L(u) - 2A(u) + (1/2) \iiint_V \left[2C_{ijnm} \varepsilon_{ij}^U \varepsilon_{ij}^u \right] dV, \quad \sigma_{ij}^U \equiv \tau_{ij}, \ \sigma_{ij}^u \equiv t_{ij} \tag{19}$$

After some transformations in Eq. 19 we can get the following equation:

$$\delta L = \delta A(U) - \delta A(u)$$

$$= \iiint_V \left\{ \left[(\tau_{ij,j} - t_{ij,j}) + P_i^V \right] \delta U_j \right\} dV - \oint\!\!\!\oint_F \left\{ \left[(\tau_{ij} n_j - t_{ij} n_j) - P_i^F \right] \delta U_i \right\} dF$$

$$+ \iiint_V \left\{ \left[t_{ij,j} - C u_i - P_i^V \right] \delta u_j \right\} dV - \oint\!\!\!\oint_F \left[(t_{ij} n_j + P_i^F) \delta u_i \right] dF$$

$$+ \left\{ \iiint_V [P_i^V \delta u_j + \oint\!\!\!\oint_F [P_i^F \delta u_i] dF \right\} = 0 \tag{20}$$

So, we established that the initial boundary problem could be formulated on the full stresses $\sigma_{ij} = \tau_{ij} - t_{ij}$ and cohesion stresses. The similar conclusion can be received after consideration of the bilinear energetic form for displacement vectors $\vec{R}$, $\vec{R}'$:

$$E(\vec{R}, \vec{R}') = \iiint_V [2\mu \varepsilon_{ij} \varepsilon'_{ij} + \lambda \theta \theta' + C u_i u'_i] dV$$

$$= \iint_F (\vec{\tau}' \vec{R}' - \vec{\sigma}' \vec{u}) dF + \iiint_V (1/C) L L_C(\vec{R}) \vec{R}' dV, \tag{21}$$

here $\theta = div \vec{R}$, $\vec{\tau} = \tau_{ij} n_j$ and $\vec{\sigma}' = \sigma'_{ij} n_j$.

Result, the boundary conditions can be formulated separately for cohesion and classical stress tensors, on the free cracks faces. In contrast to classical formulation the second order gradient theory gives the additional boundary condition, which can be formulated only respect to cohesion stresses.

To receive more clear physical results we consider problem about opening crack for isotropic body in particular, simplified double plane formulation using the following propositions: $R_i Y_i = R(x, y)$, a $R_i X_i \equiv 0$; here $\{X_i\}$, $\{Y_i\}$ are the vectors of coordinate axis. In this case we have the following variation formulation of the problem:

$$L = A - (1/2) \iint [(\mu R_{,x} R_{,x} + (2\mu + \lambda) R_{,y} R_{,y}) + C u u] dx dy.$$

Taking into account (20), (21) we can see that the stress state problem for opening crack for simplified double plane formulation is constructed as linear combination of classical (τ) and cohesion (t) stresses: $\tau = A^U r^{-1/2} Cos(\varphi/2)$, $t = A^u K_{1/2}(r\sqrt{C/(2\mu+\lambda)}Cos(\varphi/2)$, here A^U, A^u are the constants, angle φ counts out from positive axis x. This solutions are satisfied the homogeneous boundary conditions on the crack faces ($x \leq 0$; $y = 0$) and have the same asymptotes near the top of crack $r \to o$. Using these solutions and taking into account that $t = A^u K_{1/2}(r\sqrt{C/(2\mu+\lambda)}Cos(\varphi/2)$, describes the cohesion type field near top of crack, it is easy to find the nonsingular solution in the following form:

$$\sigma = (2\mu+\lambda)\left[(2/\pi)^{1/2}\sqrt{[(2\mu+\lambda)/C]^{1/2}}K_\alpha\left(r\sqrt{C/(2\mu+\lambda)}\right) - r^{-(1/2)}\ \right]Cos(\varphi/2) \tag{22}$$

где $\alpha = 1/2$, $r = \sqrt{[\mu/(2\mu+\lambda)]y^2 + x^2}$

Equation 22 defines the nonsingular stresses in a vicinity of the top of crack. These stresses have the classical asymptotical behavior on the infinity ($r \to \infty$).

Let's consider the asymptotical equation, which follows from the Eq. 22.

$$\sigma = \sigma_a(1 - e^{-ar})(ar)^{-1/2}\cos(\varphi/2) \tag{23}$$

Here $a^2 = C/E$, σ_a is the some amplitude of the stresses and $E = 2\mu + \lambda$ is the modulus of elasticity.

Note that upper and lower faces of the crack are correspond to the angles $\varphi = +\pi$ and $\varphi = -\pi$. Stress σ takes on a maximum value on the distance r_* from the top of crack, which can be found from the condition $\partial\sigma/\partial(ar) = 0$. It is easy to find $q = ar_* = 1{,}256431$. So we can define the nonclassical physical constant C from distance r_* (the length of Barenblatt zone):

$$C = q^2 E/r_*^2 = 1{,}578619\ E/r_*^2$$

The stress σ is achieved of the maximum in the point r_* near top of crack ($\varphi = 0$). Then we can write (see Eq. 23):

$$\sigma_{\max} = \sigma_a(1 - e^{-q})(q)^{-1/2} \text{ and } \sigma_a \approx 1{,}566974\sigma_{\max},\ (q = ar_* = 1{,}256431)$$

It is interesting to establish the relation between of the maximum stresses $\sigma_{\max}$ and displacements of crack faces. The displacement of crack faces can be found by integrating of equations for stresses σ:

$$\begin{aligned} v(r,\varphi) &= 2(\sigma_a/aE)(1 - e^{-ar})(ar)^{1/2} Sin(\varphi/2) \\ &= \sigma_{\max}(3{,}133948/aE)(1 - e^{-ar})(ar)^{1/2} Sin(\varphi/2) \end{aligned}$$

Dependence of the crack faces displacement, $v(r, \varphi = \pi)$ from r is shown on the Fig. 1. This dependence has, obviously, a inflection point in a vicinity of top of a crack. The coordinate of this point is root of the equation $\partial^2 v(r, \varphi = \pi)/\partial r^2 = 0$.

Let's define the crack open displacement as displacement where maximum of displacement has the inflection point:

$$\delta = 2v(r^*, \varphi = \pi) = 4(\sigma_a/aE)(1 - e^{-ar^*})(ar^*)^{1/2} \tag{24}$$

The point r^* is the root of the equation $d^2 v(r, \varphi = \pi)/dr^2 = 0$.

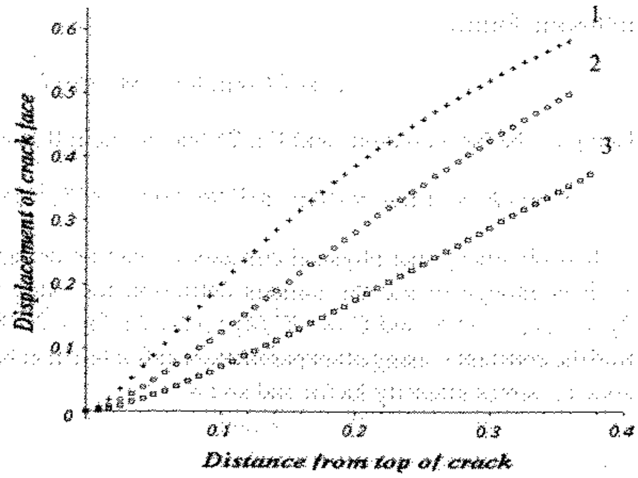


Fig. 1 Dependence of the relative crack faces displacement $\bar{v} = (1 - e^{-ar})(r)^{1/2}$ from r (curve 1—$a = 0.1$; curve 2—$a = 0.03$; curve 3—$a = 0.01$)

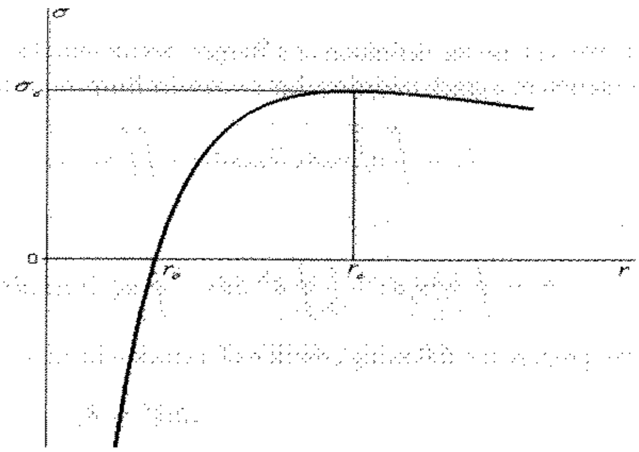


Fig. 2 Typical distribution of the interatomic interactions

Assume that $\sigma_{\max}$ is achieved of the limited stresses $\sigma_{\max} = \sigma_C$ of the material under consideration. Then, we can find from Eq. 24 limited critical value of the crack open displacement:

$$\delta_c = 6,267896(\sigma_c/aE)(1 - e^{-ar^*})(ar^*)^{1/2} \quad (25)$$

Let's note that some estimation of limited stresses σ_C from limited deformation ε_C can be received using simplified consideration of the interatomic interactions for two levels of atoms. The typical distribution of these interactions is known from quantum mechanical approach (see Fig. 2). Assume that r_0 is the equilibrium interatomic distance and r_c is the limited interatomic distance, which corresponds to theoretical ultimate stresses σ_C.

Then we can use the following equations for approximation of the typical distribution of the interatomic interactions (see Fig. 2), that is known from quantum mechanical approach:

$$\sigma = \sigma_C Sin[(\pi/2)(r - r_o)/(r_c - r_o)] = \sigma_C Sin[(\pi/2)(\varepsilon/\varepsilon_c)], \quad \text{if } r_o < r < r_c$$
$$\text{and } \sigma = 0 \quad \text{if } r_c < r$$

We interpreted value $(r - r_o)/r_o$ as tensile strain ε : $\varepsilon = (r - r_o)/r_o$ and $\varepsilon_c = (r_c - r_o)/r_o$. Using definition $E = [d\sigma/d\varepsilon]|_{\varepsilon=0}$ the ultimate theoretic strength σ_C can be found in the following forms:

$$\sigma_C = 2E(\varepsilon_C/\pi), \quad \text{or} \quad \sigma_C/E = 2\varepsilon_C/\pi$$

Using of the last equations and Eq. 25 lead to the following formula for constant C:

$$C = (E/\delta_c^2)(2\varepsilon_C/\pi)^2[(6,267896)^2/(1-e^{-q})^2(q)], \quad (q = ar_* = 1{,}256431)$$

It is obviously that physical constant C: can be defined through specific surface energy γ. It is enough to use the famous definition for value γ we can get: $2\gamma = \sigma_c\delta_c$. Then $2\gamma = (2\varepsilon_C/\pi)E\delta_c$ and $C = (E^3/4\gamma^2)(2\varepsilon_C/\pi)^4[(6,267896)^2/(1-e^{-q})^2(q)]$. It is easy to find the constant C using other parameters of fracture mechanics: the length of the Barenblatt's zone r_*, stress intensity factor and so on.

6 About criterions in fracture mechanics

1. We will use the definition of a Burgers vector introduced in Sect. 2 for formulation of the criterion of a crack initiation. Let's consider Burgers vector

$$b_i = \oint d_{ij}^{\Xi} v_m n_n \exists_{jmn} ds = \iint \Xi_{in} n_n dF = n_n \iint \Xi_{in} dF.$$

or

$$b_i = \oint \gamma_{ij}^{\Xi} s_j ds + \frac{1}{3}\oint \theta^{\Xi} s_i ds - \oint \omega_k^{\Xi} \exists_{ijk} s_j ds = (b_i)_\gamma + (b_i)_\theta + (b_i)_\omega$$

We propose the following criterion of a crack initiation

$$\|b_i\|^2 = K_b \tag{26}$$

where K_b is some critical value.

To realize this criterion we must define K_b and to propose definition of the contour of integration for calculating of the right part in Eq. 26. We propose to use the following definition for K_b:

$$K_b = (\delta_c)^2,$$

where constant δ_c defines by the Eq. 25.

As a contour of integration for calculating of the Burgers vector in a plane problem, the plane contour of circle with radius of "r^*" is proposed to use. This radius is found as root of Eq. $d^2v(r, \varphi = \pi)/dr^2 = 0$. This value has clear physical sense because it disjoints the cohesion zone in vicinity of top a crack.

2. The proposed advantage model in contrast to different variants of the gradient theories, describes not only scale affects in the volume, but also corresponding spectrum of adhesion properties. In common case (see Lurie and Belov 2005, 2006) the density of superficial energy has four components: surface tension energy; the distortion energy and the energy of torsion in the plane tangent to the surface correspondingly; and the energy of surface bending that connected with Laplace pressure. Then we can specify the specific surface energy γ and connect it with four mentioned above types of adhesion surface properties. To realize this way we must previously to find adhesion parameters using specific set of experimental investigations. This problem is not solved on present time.

Let's consider the particular Aero-Kuvshinskii's model, Eqs. 12–15 and the density of potential surface energy, which is defined by the damage. This density of energy can be interpreted as the energy of the new generated surface. Let's introduce the following functional: $\iint D_{ij}\dot{R}_i\dot{R}_j dF$, where $D_{ij} = An_in_nn_jn_m + B(\delta_{in} - n_in_n)n_jn_m$, (see Eqs. 14), and $\dot{R}_i = (\partial R_i/\partial x_j)n_j = \partial R_i/\partial n$ is the normal derivative.

Then, we can propose the following local and integral criterions of the crack stability:

Integral criterion- $\gamma \geq (1/2F)\iint D_{ij}\dot{R}_i\dot{R}_j dF$,
Local criterion- $\gamma \geq (1/2)D_{ij}\dot{R}_i\dot{R}_j$
Constant γ is the physical constant of material.

It can be proved (see Eqs. 12, 14, 16 and Lurie et al. 2005, 2006) that D_{ij} is included only in nonclassical boundary conditions at the variations of $\delta\dot{R}_i$: $D_{ij}\dot{R}_j + C_{ij}u_j = 0$, where C_{ij} is tensor of reduced modulus Using last equation we can find $\dot{R} = -D_{ki}^{-1}C_{ij}u_j$. So, dislocation corrections on the surface connected only with quadratic form of cohesion displacements and local criterion of the crack stability can be written in the form:

$$\gamma \geq (1/2)(C_{in}D_{nm}^{-1}C_{mj})u_iu_j$$

For more general case the following generalized criterion of the crack stability can be proposed: The crack becomes unstable when quadratic form of the cohesion displacement in the volume and on the surface more then some critical constant.

$$\gamma \leq (1/2V)\iiint Cu_ku_k dV + (1/2F)\iint (C_{in}D_{nm}^{-1}C_{mj})u_iu_j dF$$

3. Let's consider shortly the question about deflection of the known Hall-Petch law from experimental dates for nanocrystalline materials. The Hall-Petch's law determines dependence of the ultimate stresses of the polycrystalline materials from the grain size and has the following view

$$\tau = \tau_0 + Kd^{-1/2}$$

here τ_0 is the sliding stress, K is the physical constant

For nanocrystalline materials the regular sufficient deviation from the classical Hall-Petch law is observed. Different type attempts were undertaken to model this effect, which in detail are described in the review Gutkin and Ovidko (2003).

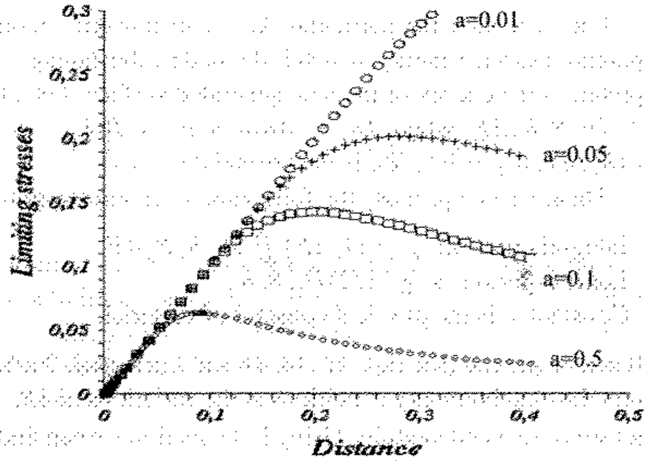
We would like to show that effect of regular deflection from Hall-Petch law can be modeled on the basis of the gradient theory of media with conserved dislocation. Really, let's consider simplified equations for shear stresses τ

$$\tau = \tau_a(1 - e^{-ar})(ar)^{-1/2}Cos(\varphi/2), \quad a^2 = C/\mu \tag{27}$$

This equation is analogous with Eq. 23 and can be received by the similar way from the simplified variant of the cohesion type model. Assume that $\tau_0 = 0$, and maximum stress of cohesion field in some point r_0 defines the start of the instability. We propose also that parameter $r_0 \equiv d$ defines the grain size. Let's consider dependence for reduced stresses $\bar{\tau} = d(1 - e^{-ad^2})$, $a^2 = C/\mu$, that follows from Eq. 26.

Curves of Fig. 3 show a deviation scope from the law of the Hall-Petch (the top asymptotic on the Fig. 3), in dependence of scale parameter a. The deviations from the law of the Hall-Petch grow with increasing of parameter $a = 0.01$; 0.05; 0.1; 0.5. In a qualitative sense shown curves quite correspond to the specified dependences for the micro-hardness (see Gutkin and Ovidko 2003), which were received by the other way and have good agreement with experimental dates if in appropriate way to select the parameter a.

Fig. 3 Effect deviation from the classical Hall–Petch law for nanocrystalline materials



So, the analysis show that, Barenblatt's hypothesis is very productive from the point of view of the theory media with conserved dislocations. On the one hand it allows to carry out expansion of the continuum mechanics methods on the fracture mechanics.

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