The adhesive and antiadhesive non-local interaction of solids

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**Abstract.** The inequalities which must be satisfied the characteristics of elastic state of the materials of contacting bodies at their adhesion (coalescence) and its absence (antiadhesion) were obtained. These are the result of the analysis of adhesion phenomena and its absence. The analysis is made on the basis of a special variant of a nonlocal theory of elasticity. Its main hypothesis is infinitely small particles of the continuous elastic medium interact with each other at finite distances with the help of many-particle potential forces. The results of using criterial inequalities were confirmed by known experimental data.

1. Introduction

When creating high-tech and science-intensive products, depending on the functions performed, there are situations when adhesion is required between contacting bodies (layered structures) or it should be absent. In the first case a composition of materials of the layered structure elements is selected, which provides its greatest strength. In the second case, antiadhesive layer or coating is used. The material of this layer (coating) should have antiadhesive properties in relation to the protected material (it should not stick together).

At the present time the industry uses a variety of experimentally tested materials with appropriate properties. At the same time, there are no criteria by which to predict theoretically the adhesive or antiadhesive properties of a particular pair of materials. This work is devoted to a partial solution of the problem of constructing such a criterion for linearly elastic materials. It is based on non-local model, which takes into account the paired and triple potential interactions of particles interacting materials at finite distances. At the same time, we use a number of assumptions about the character of these interactions of the individual particles and the contacting bodies in general.

2. Nonlocal potential interaction of particles of a continuous elastic medium

Adhesion of solids \(B_{(1)}\) and \(B_{(2)}\) is their coalescence [1]. Therefore, the antiadhesion can be called a property of a material, which is resistant to sticking of other material to it. The phenomenon of adhesion is caused by the action of Van der Waals forces between neutral particles or Coulomb forces between charged particles [2, 3] of the interacting bodies. Because of this antiadhesion (no adhesion) can be explained either by a lack of attractive forces between particles of different materials or their groups, or the occurrence of repulsive forces between them.

The continuous elastic medium is a mathematical model of real materials with their discrete atomic-molecular structure. This structure is characterized by a non-local potential interaction of
composing them particles. In the works [4–7] this property is axiomatically transferred to the interaction of particles of a continuous elastic medium.

The body \( B = B_{(1)} \cup B_{(2)} \) (\( B_{(1)} \cap B_{(2)} = \emptyset \) corresponds to a discrete structure \( N = N_{(1)} + N_{(2)} \) of material points with masses of \( m_{(1)} \) and \( m_{(2)} \), and the radius vectors \( \mathbf{r}_{(1)} \) and \( \mathbf{r}_{(2)} \). Its potential interaction energy of all particles is determined by expression [8]:

\[
U(\mathbf{r}_1, ..., \mathbf{r}_N) = U(\mathbf{r}_{(1)}, ..., \mathbf{r}_{N(1)}; \mathbf{r}_{(2)}, ..., \mathbf{r}_{N(2)}) = U_{(1)}(\mathbf{r}_{(1)}, ..., \mathbf{r}_{N(1)}) + U_{(2)}(\mathbf{r}_{(2)}, ..., \mathbf{r}_{N(2)})
\]

The first and second terms of expression determine the potential energy of the interaction of particles in the bodies \( B_{(1)} \) and \( B_{(2)} \). The third term is the potential energy of interaction between the particles, which belong to different bodies. At the same time, there are works [9] in which the adhesive interactions are not considered as volumetric (three-dimensional), but as surface (two-dimensional) interactions. To carry out the necessary calculations, we use representation of these potential energies in the form of sums of all pairs of interacting particles, their triplets, etc.

\[
U(\mathbf{r}_1, ..., \mathbf{r}_N) = \sum_{\alpha=1}^{2} \left( \sum_{i=1}^{N_{\alpha}} \sum_{j=1}^{N_{\alpha}} U^{(2)}_{(\alpha)}(\mathbf{r}_{(\alpha)i}, \mathbf{r}_{(\alpha)j}) + \sum_{i=1}^{N_{\alpha}} \sum_{j>i}^{N_{\alpha}} U^{(1)}_{(\alpha)}(\mathbf{r}_{(\alpha)i}, \mathbf{r}_{(\alpha)j}, \mathbf{r}_{(\alpha)k}) + ... \right)
\]

Here \( \alpha, \beta, \gamma = 1,2 \) is the number of the material (body), \( \beta \neq \gamma \). Generally only pair interactions of particles are considered (the first double sum in parenthesis of expression (2)) [10] with potentials such as the potential of the Lennard-Jones, London, Morse, etc, which provide the stability of the lattice structures as each of the bodies \( B_{(1)} \) and \( B_{(2)} \), as well as the combined body \( B = B_{(1)} \cup B_{(1)} \). In papers [11, 12] it was shown that the triple interactions can lead not only to the attraction of the particles, but also their repulsion. Therefore, this may contribute to the appearance of antiadhesion.

In the proposed for further consideration model, the role of particles is played by the infinitely small particles \( d B_{(\alpha)} \) of each of the bodies \( B_{(\alpha)} \) (\( \alpha = 1, 2 \)). They are obtained by a mental partition

\[
B_{(\alpha)} = \lim_{N_{(\alpha)} \to \infty} \bigcup_{n=1}^{N_{(\alpha)}} \Delta B_{(\alpha)n} = \int d B_{(\alpha)} \quad (n \neq m) \Rightarrow \Delta B_{(\alpha)m} \cap \Delta B_{(\alpha)n} = \emptyset
\]

Partitions (3) are used in the construction of integral sums in the calculation of additive characteristics of state of the solid body material \( B_{(\alpha)} \).

Also as for the discrete point systems [8], the potentials of pair and triple interactions are described by empirical functions with the parameters characteristic of the test material, or a pair of materials. These functions correspond to the conditions of thermo-dynamic system. To perform the first requirement it is assumed that partial potentials \( d^n \Psi^{(n)}_{j(a)} \) of interaction \( n \) particles (both one and different materials) are infinitely small quantities of \( n \)-th order with respect to volume \( \Delta V_{j(a)} \to 0 \) (\( j = 1, 2, ..., n \)):

\[
d^n \Psi^{(n)} = \Phi^{(n)} d V_{1(a)} d V_{2(\beta)} ... d V_{n(\gamma)}
\]

The coefficient of proportionality \( \Phi^{(n)} \) (further the potential) depends only on the relative distances \( I_{j(a)} = |\mathbf{r}_{j(a)}| \) between the interacting particles, \( \mathbf{r}_{j(a)} = \mathbf{r}_{j(\beta)} - \mathbf{r}_{(a)} \) – the radius vector of
particle $dB_{(\beta)}$ relative to the particle $dB_{(\alpha)}$ in the current configuration of the body $B = B_{(\alpha)} \cup B_{(\beta)}$.

If between any pair of particles the distance is $l_{ij(\alpha\beta)} \to \infty$, then $\Phi^{(\alpha)} \to 0$. This happens with the speed required for the convergence of all integrals.

Also, as for the discrete point systems [8], the potentials of pair and triple systems interactions of infinitely small particles of the same material, which form a continuous solid, satisfy the stability condition of specific configuration of the particle system.

For particles of the same material $\alpha = \beta$ dependence of $\Phi^{(\alpha)}$ on $l_{ij(\alpha\beta)}$ is such that the internal forces, which are generated by the deformation of the material, always keen to return it to its original state.

The interaction potentials of groups of particles of different materials, as well as the bodies themselves, can satisfy and not satisfy the condition of stability. In the first case, this corresponds to the presence of adhesion, in the second – to its absence.

As a result, the analogue of representations (1) and (2) is an expression

$$W = \frac{1}{2} \sum_{\alpha=1}^{2} \int_{V_{(\alpha)}} \Phi^{(2)}_{(\alpha\alpha)} dV_{1(\alpha)} dV_{2(\alpha)} + \frac{1}{3} \sum_{\alpha=1}^{2} \int_{V_{(\alpha)}} \Phi^{(3)}_{(\alpha\alpha\alpha)} dV_{1(\alpha)} dV_{2(\alpha)} dV_{3(\alpha)} + ...$$

$$+ \frac{1}{2} \sum_{\alpha, \beta=1}^{2} \int_{V_{(\alpha\beta)}} \Phi^{(2)}_{(\alpha\beta)} dV_{1(\alpha)} dV_{2(\beta)} + \frac{1}{3} \sum_{\alpha, \beta, \gamma=1}^{2} \int_{V_{(\alpha\beta\gamma)}} \Phi^{(3)}_{(\alpha\beta\gamma)} dV_{1(\alpha)} dV_{2(\beta)} dV_{3(\gamma)}$$

(5)

Here $\Phi^{(2)}_{(\alpha\alpha)}$, $\Phi^{(2)}_{(\alpha(\alpha\beta)} \equiv \Phi^{(2)}_{(\alpha\beta)}$, $\Phi^{(3)}_{(\alpha\alpha\alpha)}$, $\Phi^{(3)}_{(\alpha\beta\gamma)} = \Phi^{(3)}$ – are the potentials of pair and triple interactions of particles from materials with corresponding numbers; $V_{(\alpha)}$ – the area (or its volume) occupied at the time $t$ by body $B_{(\alpha)}$, $dV_{1(\alpha)}$ – volume of particle $dB_{(\alpha)}$ at this time (it is assumed that the deformation is small, so the time index $t$ is further discarded ). In this expression we restricted ourselves to taking into account no more than three-particle interactions.

In condition of absence external mechanical influences on the body $B = B_{(1)} \cup B_{(2)}$ you can obtain expressions for the energy $dW_{(1)}(\vec{r}_{(1)})$ of infinitely small particle, for example, $dB_{(1)}$:

$$dW_{(1)}(\vec{r}_{(1)}) = w_{(1)}(\vec{r}_{(1)}) dV_{(1)} = (w_{(11)} + w_{(12)}) dV_{(1)}$$

$$= \left[ \int_{V_{(1)}} \Phi^{(2)}_{(12)} dV_{(1)} + \frac{1}{2!} \int_{V_{(2)}} \Phi^{(3)}_{(12(12)} dV_{1(1)} dV_{2(1)} \right] dV_{3(1)}$$

$$+ \left[ \int_{V_{(1)}} \Phi^{(2)}_{(12)} dV_{(2)} + \frac{2}{3} \sum_{\beta, \gamma=1}^{2} \int_{V_{(\beta\gamma)}} \Phi^{(3)}_{(12(1\beta\gamma)} dV_{1(\beta)} dV_{2(\gamma)} \right] dV_{3(1)}$$

(6)

In this equation $w_{(11)}$ – is the bulk density of the potential energy, which arose due to the interaction between particles of the body $B_{(1)}$; $w_{(12)}$ – the addition to the value $w_{(11)}$, which arose due to interaction of particles of body $B_{(1)}$ with particles of body $B_{(2)}$.

The force $\vec{f}_{(1)} dV_{(1)}$ of action on the particle $dB_{(1)}$ from the environment is defined by the equality:

$$\vec{f}_{(1)} = - \nabla_{\vec{r}} w_{(1)} = - \nabla_{\vec{r}} w_{(11)} - \nabla_{\vec{r}} w_{(12)} = \vec{f}_{(11)} + \vec{f}_{(12)}$$

(7)
The force $\vec{f}_{(1)}$ d$V_{(1)}$ acts on the particle d$B_{(1)}$ only from the side of the body $B_{(1)}$, while the force $\vec{f}_{(12)}$ d$V_{(1)}$ is caused by the action on a particle d$B_{(1)}$ of all particles d$B_{(2)} \subset B_{(2)}$. The first term in the expression (7) characterizes the cohesive interaction within the body $B_{(1)}$. The second term is the adhesive interaction between the bodies $B_{(1)}$ and $B_{(2)}$. It is seen, that both types of bulk density of the potential energy of an elementary particle and also the forces acting on it, are the sums of two terms. One of them is determined by pair interactions, the second by triple ones.

In this paper, the empirical dependences $\Phi_{(2)}$ and $\Phi_{(3)}$ of potentials of pair and triple particle interactions are chosen as a Morse potential.

$$\Phi_{(\alpha \beta)}^{(2)} = \Phi_{0(\alpha \beta)}^{(2)} \varphi_{ij(\alpha \beta)}$$  \hspace{1cm} (8)

$$\Phi_{(\alpha \beta \gamma)}^{(3)} = \Phi_{0(\alpha \beta \gamma)}^{(3)} \varphi_{(12)(\alpha \beta)} \varphi_{3(\alpha \beta \gamma)}$$  \hspace{1cm} (9)

$$\varphi_{ij(\alpha \beta)} = e^{-2 \eta_{ij(\alpha \beta)}} - 2e^{-\eta_{ij(\alpha \beta)}}$$  \hspace{1cm} (10)

In equations (8) – (10) it is acceptable the coincidence $\alpha, \beta, \gamma = 1, 2$. The parameters $\beta_{(\alpha \beta)}, \Phi_{0(\alpha \beta)}^{(2)}$ and $\Phi_{0(\alpha \beta \gamma)}^{(3)}$ characterize the properties of interacting materials and are determined by the methods described in papers [4 – 7].

3. The phenomena of adhesion, antiadhesion and their modeling

To answer the question whether or not there is the adhesion between two solid materials, the interaction of two semi-infinite bodies $B_{(1)}: 0 < x < x_{(1)} < +\infty, B_{(2)}: -\infty < x_{(2)} < 0$ is considered. To simplify the mathematical reasoning and increase the visibility of their results, the bodies are mentally divided into cylindrical parts of the same infinitely small cross-section, which are perpendicular to the plane of contact $A_{(12)}: x = 0$. So we have taken into account only those interaction forces that occur between particles of different materials, which belong to the coaxial cylinders.

The distribution of the bulk density of the potential energy of interaction of the cylinder from the body $B_{(2)}$ to a particle d$B_{(1)}$, located at a distance $x_{(1)}$ from the contact surface, is given by

$$w(\eta) = \left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^6} \right) \left( \frac{1}{2} e^{-2\eta} - 2e^{-\eta} \right) - \left( \frac{\Phi_{0(12)}^{(3)}}{\beta_{(12)}^6} \right) \left( \frac{1}{2} e^{-2\eta} - 2e^{-\eta} \right)^2$$  \hspace{1cm} (11)

where $\eta = \beta_{(12)} x_{(1)}$ is a dimensionless distance.

When

$$\eta = \beta_{(12)} x_{(1)} = 0: \ w(0) = -\frac{3}{2} \left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^6} \right) + \frac{3}{2} \left( \frac{\Phi_{0(12)}^{(3)}}{\beta_{(12)}^6} \right)$$  \hspace{1cm} (12)

The distribution of the bulk density of the interaction force is determined:

$$f_{(12)} = -\frac{dw}{dx_{(1)}} = \beta_{(12)} (e^{-2\eta} - e^{-\eta}) \left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^5} \right) + 2 \left( \frac{\Phi_{0(12)}^{(3)}}{\beta_{(12)}^5} \right) \left( 2e^{-\eta} - \frac{1}{2} e^{-2\eta} \right)$$  \hspace{1cm} (13)

When
\[
x_{(1)} \to 0: \quad f_{(12)} \to = (-2 \eta) \left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^{3}} + 3 \frac{\Phi_{0(122)}^{(3)}}{\beta_{(12)}^{6}} \right)
\]

(14)

When

\[
\left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^{3}} \right) > 0 \quad \left( \frac{\Phi_{0(122)}^{(3)}}{\beta_{(12)}^{6}} \right) > 0
\]

(15)

it turns out that \( w(0) < 0 \).

At the same time, if \( dB_{(1)} \) is displaced from the contact surface by a infinitesimal distance \( x_{(1)} > 0 \), then a restoring force \( f_{(12)} \approx (-x_{(1)}) \) appears. The system \( dB_{(1)} \cup B_{(2)} \) is stable. There is adhesion.

When

\[
\left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^{3}} \right) > 0 \quad \left( \frac{\Phi_{0(122)}^{(3)}}{\beta_{(12)}^{6}} \right) < 0
\]

(16)

we get that

\[
W(0) = -\frac{3}{2 \beta_{(12)}^{3}} \left[ \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^{3}} - 3 \frac{\Phi_{0(122)}^{(3)}}{\beta_{(12)}^{6}} \right]
\]

(17)

If

\[
2 \left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^{3}} \right) < 3 \left( \frac{\Phi_{0(122)}^{(3)}}{\beta_{(12)}^{6}} \right)
\]

(18)

then \( W(0) > 0 \), and when \( x_{(1)} \to 0: \eta \to 0 \) the force \( \Delta P_{(12)} \approx (+x_{(1)}) > 0 \) is repulsive. The system \( \Delta B_{(1)} \cup B_{(2)} \) is unstable. There is no adhesion.

If

\[
\left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^{3}} \right) < 2 \left( \frac{\Phi_{0(122)}^{(3)}}{\beta_{(12)}^{6}} \right)
\]

(19)

then \( W(0) < 0 \), but when \( x_{(1)} \to 0: \eta \to 0 \) the force \( \Delta P_{(12)} \approx (+x_{(1)}) > 0 \) is repulsive. As

\[
\int_0^{+\infty} \Delta P_{(12)} \, dx_{(1)} = \int_0^{+\infty} -\frac{dW}{dx_{(1)}} \, dx_{(1)} = W(0),
\]

that is, the energy of \( W(0) \) is the result of the interaction of all particles from the cylinder in \( B_{(1)} \), then the stability of the system (\( W(0) < 0 \)) is explained by the attraction of distant particles which prevails over repulsion of neighbors.

Expressions (12) – (19) are criterial. They can be used in the theoretical verification of the presence or absence of adhesion between a given pair of materials. They can be used for selection of a material, which has good adhesion properties with respect to the specified value. For example, the selection of elements of a strong layered structure or not at all entering into a state of adhesion with it (for example, when selecting a solid lubricant material or a protective release layer).

The parameters \( \left( \frac{\Phi_{0(12)}^{(2)}}{\beta_{(12)}^{3}} \right) \) of potentials of interparticle interactions are expressed through the Young's modulus and the shift of the contacting materials. For this, the methods described in [4 – 7]
were used. As a result, conditions that provide both good adhesion and its absence are formed. Young's and shear modules of the contacting materials are selected according to these conditions. Now let \( B_{(1)} \) and \( B_{(2)} \) be two parts of the same material. We consider their cohesion. Then

\[
\beta_{(12)} = \beta_{(1)} = \beta_{(22)} = \beta > 0 \quad \Phi^{(2)}_{0(12)} = \Phi^{(2)}_{0(11)} = \Phi^{(2)}_{0(22)} = \Phi^{(2)}_0 \]

\[
\Phi^{(3)}_{0(12)} = \Phi^{(3)}_{0(11)} = \Phi^{(3)}_{0(22)} = \Phi^{(3)}_0 \]

Also known [4 – 7]:

\[
\left( \frac{\Phi^{(2)}_0}{\beta^3} \right) = \frac{E}{294\pi(1 + \nu)(1 - 2\nu)} \quad (20)
\]

\[
\left( \frac{\Phi^{(3)}_0}{\beta^6} \right) = \frac{27E}{1764\pi^2(1 + \nu)(1 - 2\nu)} \quad (21)
\]

This indicates that \( \left( \Phi^{(2)}_0 / \beta^3 \right) > 0 \), if \( \nu > -2/41 \). While \( \nu < 0.25 \): \( \Phi^{(3)}_0 / \beta^6 \). Hence, even for homogeneous materials situation with the lack of adhesion between their parts – theoretically, and therefore with weak adhesion – in actual conditions, is possible.

For example, when

\[
\nu = 0: \quad 0.0068E = \left( \frac{\Phi^{(2)}_0}{\beta^3} \right) < 3 \quad \frac{\Phi^{(3)}_0}{\beta^6} = 0.0073E < 2 \left( \frac{\Phi^{(2)}_0}{\beta^3} \right) = 0.0136E \quad (24)
\]

Hence, a material with \( \nu = 0 \) is kept in a consistent state by the attraction of particles remote from the contact surface.

There are a number of anisotropic materials, which have in one direction \( \nu \leq 0 \) (determined by the methods described in [13]), that have anti-adhesive properties: talc, graphite, molybdenum disulfides (MoS\(_2\)) and tungsten (WS\(_2\)), etc. This is taken into account in calculating the repulsive force \( \sigma_{(12)} \) for pairs: Talc – Cu, Talc – Fe, Cu – Fe. For the first pair the following is obtained: \( \sigma_{(12)} = 65 \cdot 10^9 \text{ N/m}^2 > 0 \). Copper repels talc, there is no adhesion between them. For the second pair: \( \sigma_{(12)} = 523 \cdot 10^9 \text{ N/m}^2 > 0 \). Iron repels talc, there is no adhesion. For the third pair: \( \sigma_{(12)} = -53 \cdot 10^9 \text{ N/m}^2 < 0 \). Copper attracts steel, adhesion exists. In this case, the value \( \sigma_{(12)} \) can be considered as a theoretical tensile strength of adhesive compound. As the initial characteristics of the elastic state of the contacting materials the following values of Young's modulus \( E \) and Poisson's ratio \( \nu \) were adopted: talc [14, 15]: \( E = 0.16 \cdot 10^{11} \text{ N/m}^2 \), \( \nu = 0 \); copper [16]: \( E = 1.10 \cdot 10^{11} \text{ N/m}^2 \), \( \nu = 0.31 \); iron [16]: \( E = 2.12 \cdot 10^{11} \text{ N/m}^2 \), \( \nu = 0.26 \).

The obtained conclusions correspond to the conclusions known from technical and technological practice on the adhesion interaction of the considered pairs of materials.

**4. Conclusion**

The paper offers a description of the phenomenon of adhesion in the framework of the mechanics of a continuous deformable solid, namely a special variant of a nonlocal theory of elasticity. The proposed variant has a certain advantage in describing the phenomenon of adhesion, identifying criteria for its presence or absence, despite the fact that the analogy with solid-state physics, statistical mechanics of the discrete media in the construction of the environment model is used.
A possible presence of the adhesion between two solid materials, its energy and strength, or its absence can be judged by the values of characteristics of their elastic state, for example, Young's modulus and shear. Thus, there is no need for information about the internal atomic structure and chemical composition, internal physical properties of materials. The results of the work can be applied in the calculation of the adhesive compounds and the selection of pairs of materials with good adhesion or its absence.

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