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Estimation of the driving force acting on the interface edge

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This paper introduces a simple and approximate method of calculating the elastic driving force acting on the interface in two-phase materials. The method is based on considerations of the elastic energy connected with the change in the shape of the interface. The two phases are considered to be elastically isotropic media with different elastic constants. The procedure is developed in the framework of the finite element method and is applied to the estimation of the local driving force in the case of the edge of an interface with a singular distribution of stress. The application of T-stress to the problem is suggested.

1. Introduction

Many of the physical properties of materials are determined by their microstructure, and it is of great importance to be able to predict the microstructural development. The first step toward this goal is to estimate the role of changes in the elastic strain energy that correspond to the development of the morphology in multi-phase materials. The contribution of changes in the elastic energy to the evolution of the shape of the interface is usually studied in terms of the driving force. For example, in [3, 8, 10] the elastic driving force is used to describe the rafting process in two-phase single-crystal Ni-superalloys. In the same paper, the method for numerical determination of the driving force on the interface based on the use of domain-integral techniques (known from fracture mechanics) is described and used.

The purpose of this study is to present another, very simple and approximate, procedure for the numerical determination of the driving force on the interface. This procedure is based on finite element calculations and can be applied even to cases where the stress distribution around the interface has a singular character.

Only the two-dimensional case of a two-phase elastic material is considered. In the following, we assume that two dissimilar materials are perfectly bonded together along the interface, i.e., we assume continuity of the tractions and displacements across the boundary and that the driving force is caused by changes in the elastic strain energy.

2. Energy-rate analysis

An elastic two-phase body subjected to loads and containing an extending second phase releases energy at a rate G (that is, G is the energy per unit area of the new second phase area generated). The driving force G (or the energy release rate) thus describes the effect of a perturbation of the morphology of the second phase on the total energy E^T of the two-phase system.

Let us consider a body of arbitrary shape with A the region of the second phase, see Fig. 1. The body is subjected to an arbitrary system of applied forces F_i on the boundary portion S_1 and displacements u_k on the remaining portion S_2. In the following, the thickness of the body t is assume to be unit, i.e., $t = 1$.

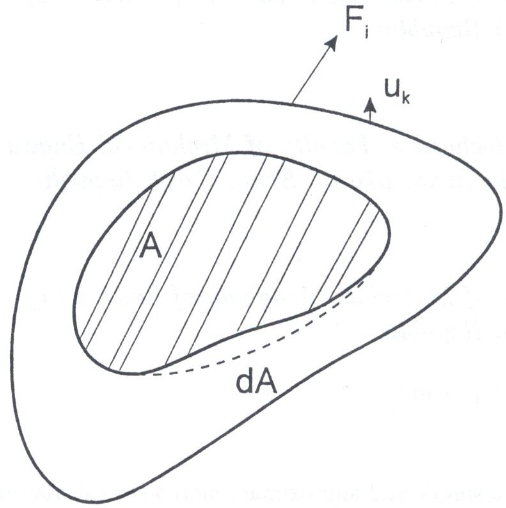

Fig. 1. The extension dA of the second phase A in an arbitrary two phase body. The boundary conditions are specified by distribution of the tractions F_i on the part of the boundary and by the displacements u_k given on the other part of the boundary of the body.

The energy G available for an increment of extension of the second phase area dA, is given by the equation

$$G = \frac{E^T(A + \mathrm{d}A) - E^T(A)}{\mathrm{d}A}\,, \tag{1}$$

and is supplied by the work done by external forces and the release of the total strain energy stored in the body. In the case of the body shown in Fig. 1, this is

$$G = F_i \frac{\mathrm{d}u_i}{\mathrm{d}A} - \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}A}(F_i u_i)\,, \tag{2}$$

wherein u_i is the displacement of the force F_i in the direction of application, and the repeated-suffix summation convention is used.

This equation can be used for the determination of the energy release rate G. Either F_i or u_i is given for each load point i and the corresponding u_i or F_i must be determined in order to compute the derivatives.

Note that for a system of constant applied forces only, all F_i = constant and Eq. 2 simplifies to

$$G = \frac{1}{2} F_i \frac{\mathrm{d}u_i}{\mathrm{d}A}\,. \tag{3}$$

For constant applied displacements, u_i = const., it holds that

$$G = -\frac{1}{2} u_i \frac{\mathrm{d}F_i}{\mathrm{d}A}\,. \tag{4}$$

The application of Eqs. 1–4 to the estimation of the driving force G is straightforward: the value of G for a particular two-phase morphology can be obtained from a separate finite element analysis of the problem: two configurations differing by a small amount $\mathrm{d}A$ are used to represent the virtual second phase extension, and the difference in strain energy stored is estimated. However, this procedure is not preferred since the boundary value problem must be solved twice, and it is used in the present paper to test the accuracy of the other numerical methods. A procedure which evaluates the driving force G from a single finite element analysis is suggested in the next paragraph.

2.1. APPROXIMATE PROCEDURE FOR THE EVALUATION OF G

Figure 2a shows a body composed of two materials (phases) M_1 and M_2 with their interface along the line L. Lines L^+ and L^- are parallel to the interface L with the position of L^+ corresponding to the interface after the first phase M_1 extension, see Fig. 2b. Further, let $\mathrm{d}A^+$ and $\mathrm{d}A^-$ denote the areas between lines L and L^+ and L and L^- respectively. Let $\mathrm{d}E^+$ and $\mathrm{d}E^-$ represent the strain energies corresponding to the areas $\mathrm{d}A^+$ and $\mathrm{d}A^-$, and further, let $\mathrm{d}A^+ = \mathrm{d}A^- = \mathrm{d}A$. The initial total area of the first phase M_1 (second phase M_2) is $A_1 + \mathrm{d}A^-(A_2 + \mathrm{d}A^+)$.

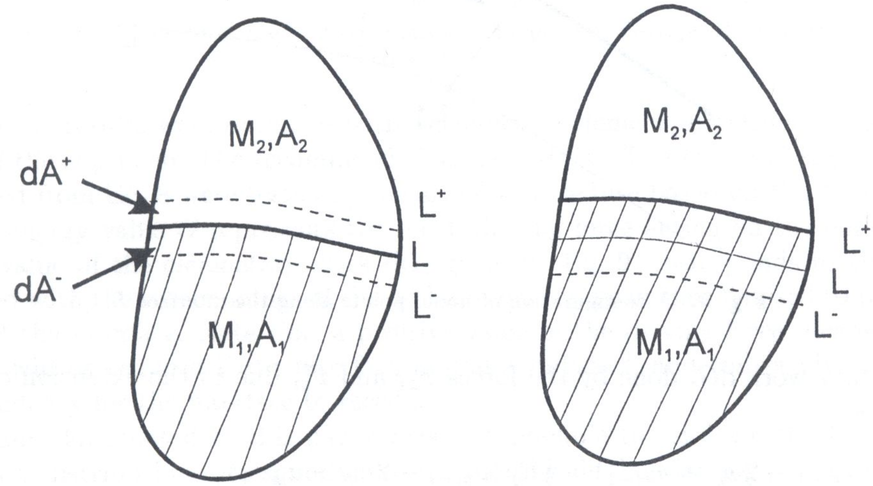

Fig. 2. A two phase body composed of two materials, M_1 and M_2: a) the initial position of the interface along the line L, b) the interface along the line L^+ after the extension of the first phase M_1.

The total strain energy E^T of the body with the initial interface position (Fig. 2a) can be expressed as a sum of terms corresponding to the separate parts of the total area A, namely

$$E^T = E(A_1) + E(A_2) + \mathrm{d}E^+(\mathrm{d}A) + \mathrm{d}E^-(\mathrm{d}A)\,. \tag{5}$$

Similarly, in the case of the interface extension (Fig. 2b), it is

$$\bar{E}^T = \bar{E}(A_1) + \bar{E}(A_2) + \mathrm{d}\bar{E}^+(\mathrm{d}A) + \mathrm{d}\bar{E}^-(\mathrm{d}A)\,, \tag{6}$$

wherein the symbol $\bar{E}$ means the strain energy corresponding to the situation with the extended first phase M_1. If

$$\mathrm{d}A^+ = \mathrm{d}A^- = \mathrm{d}A \ll A_1, A_2\,, \tag{7}$$

then G is given by [5]

$$G \cong \frac{\mathrm{d}E^-(\mathrm{d}A) - \mathrm{d}E^+(\mathrm{d}A)}{\mathrm{d}A}\,. \tag{8}$$

The energy terms in Eq. 8, $\mathrm{d}E^+(\mathrm{d}A)$ and $\mathrm{d}E^-(\mathrm{d}A)$ can be estimated directly from the results of a single finite element analysis.

2.2. Procedure for the estimating strain energy terms $\mathrm{d}E^+$and $\mathrm{d}E^-$

In this section an approximate procedure for obtaining the terms $\mathrm{d}E^+(\mathrm{d}A)$ and $\mathrm{d}E^-(\mathrm{d}A)$, see Eq. 8, is suggested. The procedure is outlined for 4-noded quadrilateral elements and can be extended to higher-type elements.

Consider a configuration of finite elements around the interface L , as shown in Fig. 3. Let F_{xi} and F_{yi} be nodal forces corresponding to the i-th nodal point on the interface and computed using the elements nearest to and around that i-th nodal point and u_{xi} and u_{yi} be the resultant nodal displacements in the x and y direction. Correspondingly, let u_{xi+1} and u_{yi+1} and u_{xi-1} and u_{yi-1} be the respective displacements of the nodal points $i+1$ and $i-1$ lying on the curves L^+ and L^-.

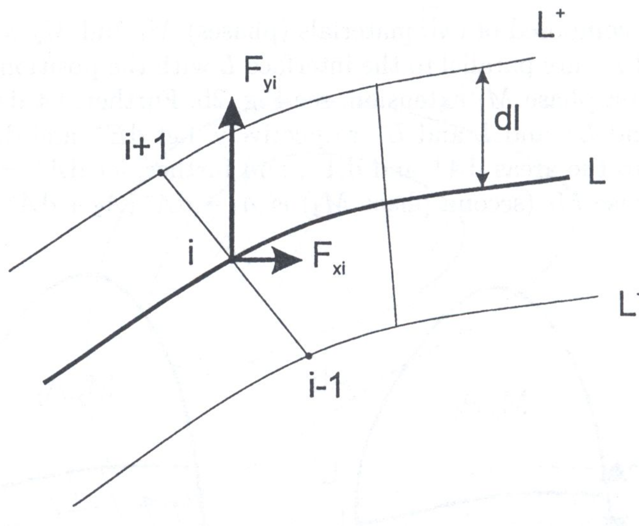

Fig. 3. A configuration of nodal points along the interface L.

The elementary work $\mathrm{d}G_i$ done by the forces F_{xi} and F_{yi} due to the extension of the interface is then given by

$$\mathrm{d}G_i \approx \tfrac{1}{2}F_{xi}(u_{xi+1} - 2u_{xi} + u_{xi-1}) + \tfrac{1}{2}F_{yi}(u_{yi+1} - 2u_{yi} + u_{yi-1}) \,, \tag{9}$$

and the corresponding total driving force G can be expressed as the sum over all the nodal points of the terms corresponding to the interface L, divided by the area $\mathrm{d}A$, corresponding to the phase extension, i.e.,

$$G \approx \sum_i \frac{\mathrm{d}G_i}{\mathrm{d}A} \,, \tag{10}$$

The procedure can be extended to higher order elements using the analogy to calculations of the crack driving force, see, e.g. [9].

Note that the estimation of the driving force is always identified with a virtual phase extension $\mathrm{d}A$ and that the exact value of G must be estimated in the limit as $\mathrm{d}A \to 0$.

To test the accuracy and reliability of the suggested procedure, extensive computational time was devoted to studying the convergence of the method. The calculations were performed with a two-phase plate specimen, see Fig. 4, and Young's modulus E_1 and E_2 of both materials were taken from the interval $0.1 < E_1/E_2 < 10.0$. It can be concluded from numerical calculations performed on four-noded elements that G converges to a constant value as $\mathrm{d}l \to 0$ (i.e., $\mathrm{d}A \to 0$), but no general rule for estimating the proper value of $\mathrm{d}l$ has been found. On the other hand, for the approximate estimation of G with an error of up to 10%, results can be obtained even with a relatively coarse mesh in the vicinity of the interface. In the case of the plate specimen (Fig. 4),

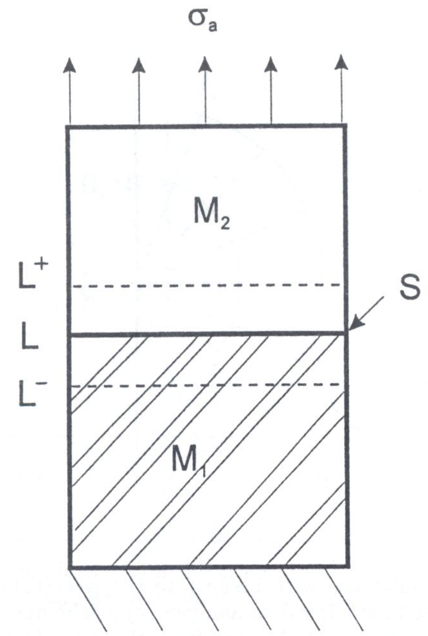

Fig. 4. Two phase specimen used for the analysis. The point S corresponds to stress singularity concentrator.

the corresponding results were obtained with an interface element dimension dl up to 5% of the total length of the specimen. The recommended value of dl is 1% of the total specimen length.The results obtained from Eq. 8 were tested by means of a procedure based on Eq. 3 in all cases.

The strain energy value G represents the mean driving force acting on the entire interface. In contrast, the value of the elementary work dG_i given by Eq. 9, corresponds to the local driving force connected with the surroundings of the nodal point i and can thus be used to predict the local morphology of the interface. Note that a positive value of the driving force means that the total elastic energy will be reduced if the interface migrates outward, and conversely, a negative value indicates a tendency for the interface to recede.

The procedure formulated in this paper makes it possible to estimate the local driving force even if the stress distribution corresponding to the interface is singular, e.g., in the case of the edge of the interface, see Fig. 4.

3. Estimation of the driving force near a stress singularity

The free edge of the interface S (see Fig. 4) represents a special case of a bi-material wedge. Due to the discontinuities of the material and its geometry at the point S the stress distribution around S is singular and for $r \to 0$ it is

$$\sigma_{ij} = \sum_n K_n r^{-\lambda_n} f_{ij}^{(n)}(\ldots\varphi,\ldots\lambda_n,\ldots) \tag{11}$$

wherein (r,φ) are the polar coordinates with the origin at the singularity point S; λ_n is called the stress singularity exponent $(0 < \lambda_n < 1)$; K_n are the stress intensity factors of the bi-material wedge; and $f_{ij}(\ldots\varphi,\ldots\lambda_n,\ldots)$ are known functions, see, e.g., [2]. The singularity exponents λ_n depend on the elastic constants of the two media M_1, M_2 and on the orientation of the interface with respect to the free surface, i.e., on the angle δ, see Fig. 5a. On the other hand, the stress intensity factors K_n depend on the total geometry and dimensions of the body, the boundary conditions and the loading. Values of the stress singularity exponents λ_n can be obtained for different angles δ and different materials by solving a certain transcendental equation resulting from an analysis based

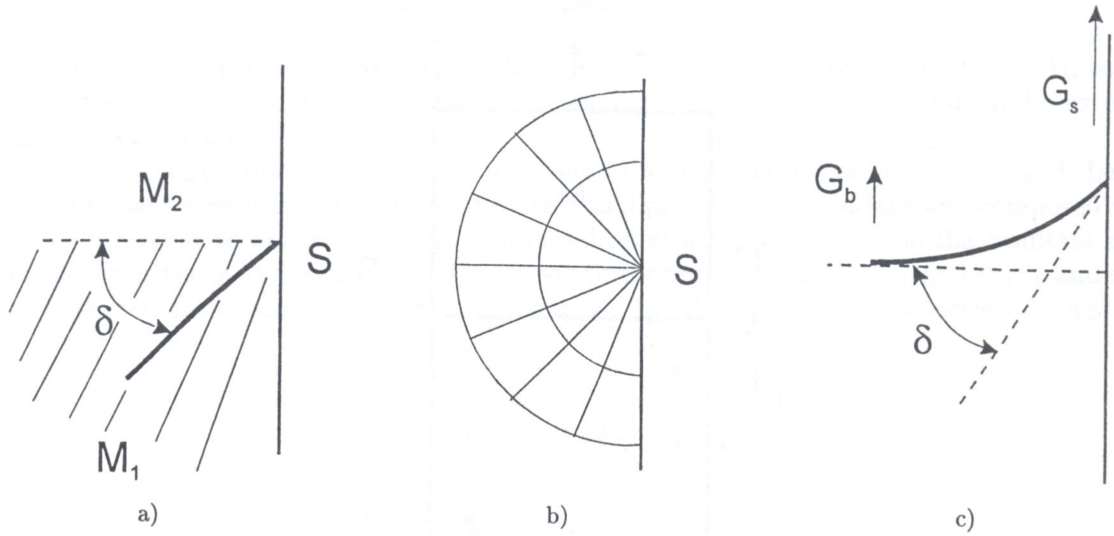

Fig. 5. a) the orientation of the interface with respect to the free surface as given by the angle δ, b) the detail of the finite element mesh used for numerical analysis, c) a schematic development of the interface. The dashed line corresponds to initial position of the interface, the solid line answers to the interface after the extension of the first phase.

on the Airy stress function, see [2, 4]. Generally, the solution of this equation can yield complex numbers, and only the values where $0 < Re(\lambda_n) < 1$ correspond to stress singularity. The values of the stress intensity factor K_n can be obtained by comparing the asymptotic solution for stress components, see Eq. 11, with the corresponding finite element results [7].

Knowledge of the values of K_n and λ_n is of great significance when determining the critical stress corresponding to the initiation of a crak at point S. The corresponding critical stress value depends on both sets of parameters [6].

In the following, the above analysis is applied to the configuration depicted in Fig. 4. First, the values of the stress singularity exponents λ_n that correspond to the given configuration (i.e., for $\delta = 0$, see Figs. 4 and 5) are calculated, see Table 1. Note that for this configuration and combination of materials there is just one real solution for $\lambda = \lambda_1$ in the interval $0 < \lambda < 1$, i.e., only one stress singularity exists.

Table 1. Stress singularity exponent λ corresponding to the configuration in Fig.4.

E_1/E_2 :	1	2	3	4	5	6	7	8	9	10
plane stress	–	.027	.060	.086	.106	.122	.134	.144	.153	.160
plane strain	–	.037	.080	.113	.135	.155	.170	.181	.191	.199

It follows further from the analysis that depending on the orientation of the interface (i.e., on the angle δ, see Fig. 5a) there exists either just one real solution $\lambda_1 = \lambda$ or no solution for λ at all in the interval $0 < Re(\lambda) < 1$. This is shown in Fig. 6 for the special case of the combination of materials $E_1/E_2 = 5$.

Further, a numerical analysis of the problem corresponding to Fig. 4 has been performed by means of the finite element system ANSYS [1] and the corresponding values of the stress intensity factors $K_{\mathrm{I}} = K$ were obtained. The details of the finite element mesh used for this calculation are presented in Fig. 5b.

In order to estimate the possible development of the morphology of the interface the free surface, the elementary work $\mathrm{d}G_s$ (see Eq. 9) corresponding to the region around the point S must be evaluated. Due to the stress singularity at the point S, the resultant nodal forces tend to infinity and the procedure outlined in Sec. 2 must be modified.

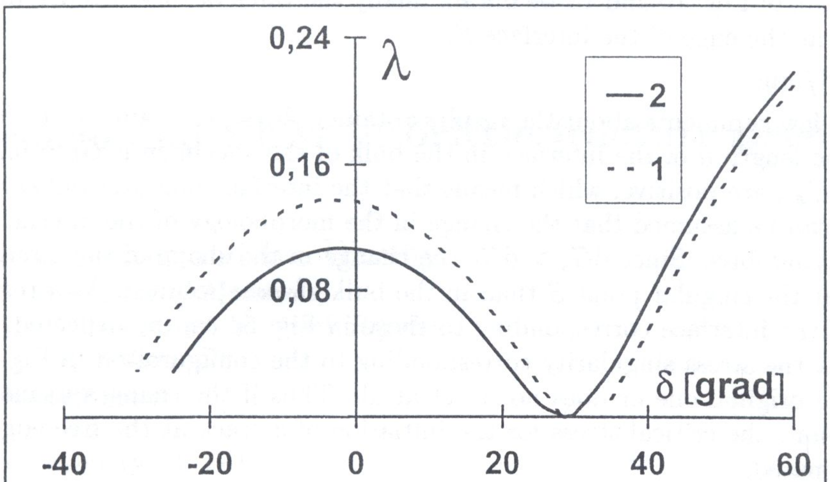

Fig. 6. Dependence of the stress singularity λ on the orientation of the interface as given by the angle δ. The solid line corresponds to plane stress, the dashed line to plane strain. The results corresponds to $E_1/E_2 = 5$.

In the following it is assumed that the deciding variable for the determination of $\mathrm{d}G_s$ is the mean stress $\bar{\sigma}_{ij}$ averaged over a certain length d along the interface, i.e., (see Fig. 5).

$$\bar{\sigma}_{ij} = \frac{1}{d}\int_0^d \sigma_{ij}(\varphi = 0)\,\mathrm{d}r\,. \tag{12}$$

Using Eq. 11 yields

$$\bar{\sigma}_{xy} = H_{xy}\frac{d^{-\lambda}}{1-\lambda}\,, \qquad \bar{\sigma}_{yy} = H_{yy}\frac{d^{-\lambda}}{1-\lambda}\,. \tag{13}$$

The total forces corresponding to the region d at the edge of the interface can then be written as

$$\bar{F}_x = \bar{\sigma}_{xy} d\,t = H_{xy}\frac{d^{1-\lambda}}{1-\lambda}\,, \qquad \bar{F}_x = \bar{\sigma}_{yy} d\,t = H_{yy}\frac{d^{1-\lambda}}{1-\lambda}\,, \tag{14}$$

wherein $t = 1$ is the thickness of the specimen. Using Eq. 9 the elementary work $\mathrm{d}G_s$ corresponding to the length d of the interface is given by

$$\mathrm{d}G_s = \tfrac{1}{2}\bar{F}_x(u_{xs+1} - 2u_{xs} + u_{xs-1}) + \tfrac{1}{2}\bar{F}_y(u_{ys+1} - 2u_{ys} + u_{ys-1})\,, \tag{15}$$

wherein the nodal point s correspond to the edge of the interface S .

Note that from a physical point of view it is reasonable to assume that the length d is a material constant and corresponds to the grain size of the materials under consideration.

Let us consider as an example the configuration corresponding to Fig. 4, and let us assume that $E_1/E_2 = 5$. According to Fig. 6, $\lambda = 0.135$ for $\delta = 0$. Furthermore, it follows from a numerical analysis performed by the finite element method (the specimen is loaded by applied stress $\sigma_{\mathrm{appl}} = 100$ MPa, and we consider plane strain approximation) and Eqs. 13 and 14 that

$$H_{xy} = 24.9\ \mathrm{MPa\,mm}^{\lambda}\,, \quad H_{yy} = 133.2\ \mathrm{MPa\,mm}^{\lambda}\,.$$

If we assumed that $d = 0.10$ mm then

$$\bar{F}_x = 3.93\ \mathrm{N}\,, \quad \bar{F}_y = 21.01\ \mathrm{N}$$

and by application of Eqs. 10 and 15 we obtain finally the value of the local driving force G_s acting on the region d at the edge of the interface S,

$$G_s = 0.243 \text{ N/mm}.$$

Let us add a few comments about the results obtained. First, the value of the local driving force G_b acting on the length d of the interface in the bulk of the specimen is $G_b = 0.091$ N/mm. Both values, G_b and G_s , are positive, which means that the interface migrates outward into the region M_2. Second, it can be assumed that the change in the morphology of the interface depends on the value of the driving force. Since $\mathrm{d}G_s > \mathrm{d}G_b$ the change in the shape of the interface will be more pronounced near the singular point S than in the bulk of the specimen. As a result developments of the shape of the interface corresponding to those in Fig. 5c can be expected. Third, it follows from Fig. 6 that the stress singularity corresponding to the configuration in Fig. 5c (for $\delta > 0$) is weaker than the original one or does not exist at all. Thus if the changes in morphology are not taken into account, the critical stress for the initiation of a crack at the free edge of the interface will be overestimated.

Note that to study the development of the morphology of the interface in cases where $\delta \neq 0$ it is necessary to take into account a non-singular constant stress term corresponding to $\lambda = 0$. The existence of this term follows from the analysis of problem using the Airy stress function [2]. The constant stress term corresponds to the T-stress known from linear elastic fracture mechanics. A more precise discussion of this point is beyond the scope of this paper.

4. Conclusions

1. Based on energy considerations, a procedure for the approximate evaluation of the interface driving force is presented.
2. The procedure makes possible the estimation of changes in the morphology of the interface under arbitrary boundary conditions.
3. The procedure has been tested on a two-phase plate specimen and applied to the case of singular stress distribution.
4. In the general case of the geometry of the interface the existence of a constant T stress term must be taken into account.

Acknowledgements

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