On propagation of interface cracks parallel to free boundaries in relation to delamination of multilayered coatings

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Abstract. The problem of a crack propagation in multilayered coating either between the individual layers, or between the whole package forming the coating and substrate (possibly also non-uniform) is considered. According to the model the delaminated part of the coating is treated as a plate with a special attention given to the boundary conditions, which are supposed to be of the elastic clamping type, which means that the angle of rotation at the clamping point is related to the acting bending moment at that point. The generalized model of elastic clamping is also considered in the frame of which it is supposed that components of displacements and angle of rotation at the clamping point are related to the acting total force and total moment by means of 3x3 matrix of elastic coefficients. Several variants of analytical models to determine the coefficients of this 3x3 matrix were considered and discussed. The case of non-uniform (multi-layered) coating is considered with a special attention paid to analysis of the influence of the relative dimensions involved, such as the individual layer and the multilayer coating thicknesses, distance from the crack to the free surface, crack length.
Using the obtained solution the problem on buckling of the delaminated coatings is addressed. It has been shown that for a wide range of parameters even for anisotropic and multilayered structures the ratio of the obtained critical stress and the critical stress of a rigidly clamped plate is determined by a single nondimensional parameter, which is a combination of the elastic constants of the coating and substrate, and the ratio of the delamination length to the coating thickness. The analytical results correlate well with the results obtained using the numerical calculations.

Keywords. Interface crack, Multilayered coatings, Delamination, Elastic clamping, Buckling

1. Introduction

Problems related to propagation of interface cracks have been investigated widely due to importance for industry. Lately they appealed additional interest owing to applications in micro- and nano-electronics, biology, medicine. The problems were addressed by many authors by using both analytical and numerical approaches e.g. [1-10]. In [2], [3], in particular, the problem of stability loss of coating delaminated from rectilinear rigid substrate was solved. The critical stress, magnitude of deflection [2], [3], and energy release rates along and across the delamination front were found. The delaminated part of coating was considered as a clamped plate, which corresponds to rigid substrates. However, detailed studies yield that, from the one hand, the condition of rigid clamping are not satisfied exactly even for absolutely rigid substrates [5], and, from the other hand, on the base of numerical calculations it is said [6], [7] that even for substrates tree times softer then coating the condition of rigid clamping yields acceptable errors. In our opinion the last statement has to be accepted with cautions, because the influence of delamination size, importance of which being confirmed by other studies [5], [8], was not investigated in [6].

Influence of the substrate rigidity was studied by [4-6], however without paying attention to the influence of the delamination width to the critical stress. The analysis of influence of both substrate compliance and delamination width on the critical stress was performed in [5]. The delamination was modeled by a plate, with boundary condition corresponding to generalized elastic clamping, i.e. magnitudes of tangential displacements and gradient of deflection of the clamped edges were supposed to be proportional to tangential force and bending moment acting at the points of clamping. The coefficients of elastic clamping depending on two mentioned parameters were calculated by solving numerically a system of integral equations [9].

Here, as well as in [9-12] the attempts were made to estimate the coefficients of elastic clamping analytically, and semi-analytically.

2. Problem formulation

Consider elastic half-plane (substrate) with adjusted layer (coating) of thickness h having elastic properties, different from the properties of substrate. The layer is perfectly glued to the half-plane everywhere except a section of length, $2b$, along which it is delaminated. The Cartesian coordinate system is chosen with x-axis being parallel the half-plane boundary, and y-axis coinciding with its external normal, the origin of the coordinate frame coinciding with the delamination centre. Thus the half-plane occupies area $y < -h/2$, the layer does $-h/2 < y < h/2$, the delamination does $-b < x < b,\ y = -h/2$. The Young moduli and Poisson ratios of the coating and substrate are E, ν, E_s, ν_s, respectively. The layer is assumed to be subjected to the tensile eigenstrain causing compressive stresses, σ_0, acting along the boundary. Such a situation takes place while heating the system in question if thermal extension of the layer is higher than the one of the half-plane. On reaching by the compressive stress some particular level of σ_{cr}, the system loses stability and the layer bends (Figure 1). The problem is to find the value of stress, $\sigma_0 = \sigma_{cr}$, corresponding to the loss of stability

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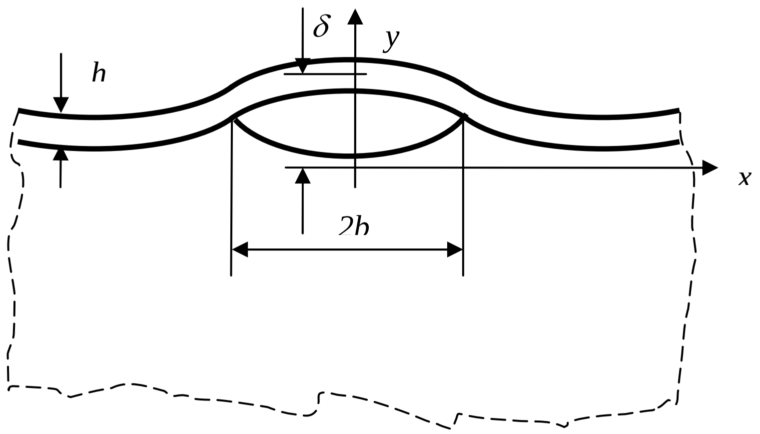

Fig. 1. Geometrical configuration.

The problem was solved in [6] numerically, using FEM, the value of σ_{cr} being presented as products of corresponding values, calculated for the clamped plane σ_0^{cr} and a coefficient γ_σ

$$\sigma^{cr} = \sigma_0^{cr} \gamma_\sigma \tag{1}$$

Magnitude of σ_0^{cr} may be calculated using elementary methods. Thus for the clamped plate of length $2b_0$ the critical stress is [13]:

$$\sigma_0^{cr} = \frac{\pi^2 h^2 E^*}{12 b_0^2} \qquad E^* = \frac{E}{1-\nu^2} \tag{2}$$

In [9-10] and here estimations for coefficient γ_σ are obtained with the help of the theory of plates.

3. Model of simple elastic clamping

In the framework of von Karman theory the plate deflection is

$$E^* \frac{h^3}{12} v^{IV}(x) + \sigma(x) h v''(x) = 0 \tag{3}$$

Here $\sigma(x)$ is the compressive stress within the cross-section of the coating. It should be noted that this stress is generally differ from σ_0 due to relaxation caused by curving of the delaminated part of the coating. For $-b < y < b$, $\sigma(x) = \sigma^{cr} = const$ the general solution of Eq. (3) is

$$v(x) = A_1 \cos kx + A_2, \ |x| < b \tag{4}$$

$$k = \sqrt{\frac{12\sigma^{cr}}{E^* h^2}} \tag{5}$$

Here constants A_i need to be determined from the boundary conditions. As a variant of the solution it may be suggested that the delaminated section of coating could be treated as a plate with elastically clamped ends. Condition of elastic clamping at points $x = \pm b$ is

$$v'(x)\big|_{x=b} = hd\, v''(x)\big|_{x=b} \tag{6}$$

Here hd is the coefficient of proportionality between the angle of the plate at clamping and the second derivative of the displacement (proportional, in turn, to the bending moment, acting at this point); d is a dimensionless coefficient that can be not determined in the frame of elementary theory. The presence of plate thickness h is due to necessity of adjusting dimensions: this parameter is the only one of the dimension of length in the model, because the clamping stiffness may not depend on the plate size b (for more information see [9-10]). Substitution of Eq. (4) into Eq. (6) yields

$$\tan kb + khd = 0 \tag{7}$$

The expression for coefficient d were obtained in [11] on the base of the model where the coating was considered as a plate and the substrate as half-plane. The solution was found with the help of Fourier transform and Wiener-Hopf technique. By neglecting the action of shear stress it was found

$$d = d_0 \sqrt[3]{E^*/E_s^*}, \ d_0 = 2^{2/3} 3^{-5/6} \approx 0{,}636 \tag{8}$$

Here

$$E^* = E/(1-\nu^2) \tag{9}$$

For rigid clamping

$$k_0 = \frac{\pi}{b} \tag{10}$$

Substituting Eq. (1), Eq. (5), Eq. (8), Eq. (10) into Eq. (7) gives

$$\tan \pi\sqrt{\gamma_\sigma} + d_0\pi\beta\sqrt{\gamma_\sigma} = 0 \tag{11}$$

Here

$$\beta = (h/b)\sqrt[3]{E^*/E_s^*} \tag{12}$$

Dependence of γ_σ on β according to this model is also presented on Figure 2. The most probable reason for the slight systematical divergence seems to be in underestimation of the critical stresses in numerical calculations.

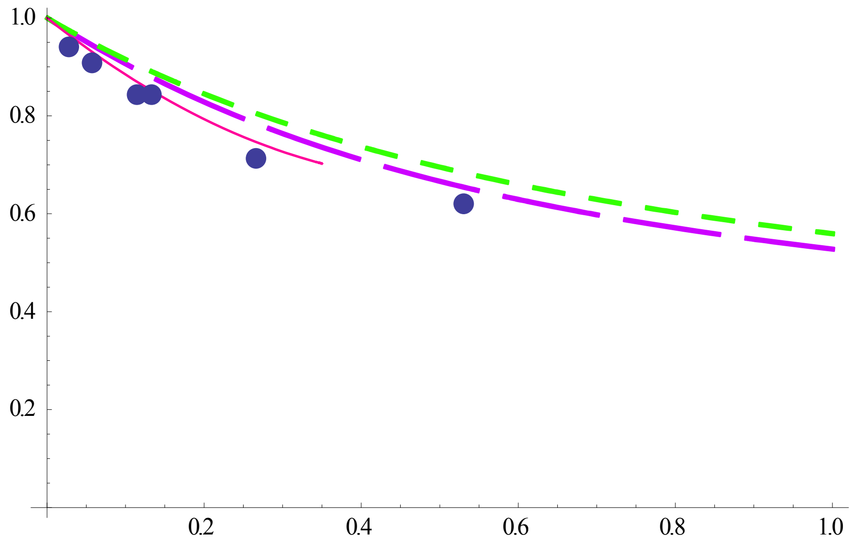

Figure 2. Dependence of relative critical stress on geometrical and elastic parameters: purple dashed line – solution Eq. (11); green dashed line (short dashes) – Eq. (18); solid red thin line – Eq. (26); dots – numerical solution [9]

4. Generalization for the case of multilayered coating and substrate

The above model is easily generalized for the case of anisotropic (orthotropic) and multilayered coating and substrate. For anisotropic phases all the above formulae remain valid with replacing the values of effective moduli Eq. (9) of coating and substrate by the values corresponding to anisotropic media. Thus for substrate instead of the second formula of Eq. (9) we have

$$E_s^* = 2\left\{\beta_{22}\left[\beta_{66} + 2\left(\beta_{11} + \sqrt{\beta_{11}\beta_{22}}\right)\right]\right\}^{-1/2} \tag{13}$$

Here β_{ij} are components of compliance tensor written in matrix form (eg [14]), axis x_1 is directed along layering, axis x_2 is directed along the normal.

For anisotropic (orthotropic) coating modulus E^* should simply be replaced with the longitudinal modulus: $E^* = E_{22}$.

For multilayered structures, if the thickness of individual layers are much less than the characteristic size of delaminated part of coating, the layered structure may be described as an effective homogeneous anisotropic media [15]. The value of effective longitudinal modulus of coating may be calculated as an averaged over the individual layers forming its delaminated part

$$E^* = \frac{\sum E_i^* h_i}{\sum h_i} \tag{14}$$

Here E_i^*, h_i are elastic moduli and thicknesses of the individual layers.

Similarly, for the multilayered substrate the effective elastic constants may be expressed as follows

$$c_{11}^* = \frac{\sum c_i^{11} h_i}{\sum h_i} \qquad c_{12}^* = \frac{\sum c_i^{12} h_i}{\sum h_i} \qquad c_{22}^* = \frac{\sum h_i / c_i^{22}}{\sum h_i} \qquad c_{66}^* = \frac{\sum h_i / c_i^{66}}{\sum h_i} \tag{15}$$

Coefficients of matrix of elastic compliance β_{ij} to be substituted to (13) are obtained from here by inversing the matrix of elastic constants.

$$\beta_{11} = \frac{c_{22}^*}{c_{11}^* c_{22}^* - c_{12}^{*\,2}} \qquad \beta_{22} = \frac{c_{11}^*}{c_{11}^* c_{22}^* - c_{12}^{*\,2}} \qquad \beta_{66} = c_{66}^{*\,-1} \tag{16}$$

It is worth to note, that the above formulae describe the crack propagation in multilayered coating both between the individual layers and between the whole package forming the coating and substrate. The difference consists in accounting the particular number of layers while calculating the effective properties Eq. (14), Eq. (15).

5. Model of generalized elastic clamping

The model of elastic clamping may be generalized in order to account the influence of longitudinal force on the boundary conditions. Such a model was used by [5] for finding the critical stress of buckling of the delaminated coating. In the frame of that model it is supposed that longitudinal displacement u and angle of rotation are linear function of longitudinal force F and bending moment M acting at the point of clamping

$$\begin{aligned} EU_0 &= a_{11}F + a_{12}h^{-1}M \\ E\frac{dV_0}{dx} &= a_{21}h^{-1}F + a_{22}h^{-2}M \end{aligned} \tag{17}$$

Although condition of elastic clamping Eq. (6) was proven to be asymptotically correct [16], and other terms might be beyond the accuracy of beam (plate) theory, accounting for additional terms in Eq. (17) may be useful in numerical calculations.

The direct application of boundary condition Eq. (17) to Eq. (4) is impossible due to presence of unknown parameter F, which, however, may be found by solving the equation for longitudinal displacement u , simultaneously with Eq. (3). That was done in [5] with the final result for the critical stress after writing it in the form convenient for our purposes being:

$$\frac{12b}{\pi h\sqrt{\gamma_\sigma}}\tan\pi\sqrt{\gamma_\sigma}+a_{22}-\frac{a_{12}^2}{1+a_{11}}=0 \tag{18}$$

The coefficient of symmetric matrix a_{ij} of elastic clamping were calculated in [5] by numerical solving of a system of integral equations as functions of ratio of moduli of coating and substrate and ratio of coating thickness to the delamination length.

Taking into account that according to Eq. (12)

$$a_{22}=12d_0\sqrt[3]{E^*/E_S^*} \tag{19}$$

expression Eq. (18) differ from Eq. (11) only by its last term, which is usually not large; nevertheless its accounting leads to (slight, but systematic) deviation of the results from the master curve, obtained by using more simple Eq. (11).

Dependence of γ_σ on β according to this model is also presented on Fig. 2, coefficient a_{11} was calculated with the help of the first formula of Eq. (20) for $E^*/E_S^*=1$. If the initial surface is curved, then in addition to longitudinal force and bending moment, transverse force N appears at the clamping point. Hence, condition Eq. (17) may be generalized:

$$\begin{aligned} EU_0 &= a_{11}F+a_{12}h^{-1}M+a_{13}N \\ E\frac{dV_0}{dx} &= a_{21}h^{-1}F+a_{22}h^{-2}M+a_{23}h^{-1}M \\ EV_0 &= a_{13}F+a_{23}h^{-1}M+a_{33}N \end{aligned} \tag{20}$$

Here 3x3 matrix a_{ij} may be called the extended matrix of coefficient of elastic clamping. Calculating coefficients of the extended matrix a_{ij} may become useful for studying delamination and buckling of initially curved coatings.

6. Calculating coefficients of matrix of elastic clamping

Coefficients of matrix (20) were calculated in [4] for a particular geometric parameters numerically, and in [5] by numerical solving a system of integral equations for various ratios geometric parameters and moduli. However it is desirable to have an asymptotical, or at least, approximating formulae.

Formulae for a_{22} were obtained in [11] on the base of the model where the coating was considered as a plate and the substrate as half-plane by using Fourier transformation and Wiener-Hopf technique. The value is given by Eq. (8), Eq. (19). The value of a_{23} were found (ibid.) to be

$$a_{23}=2^{7/3}3^{-2/3}\left(E/E_S\right)^{2/3}=2.52\left(E/E_S\right)^{2/3} \tag{21}$$

Coefficients a_{11}, a_{12} (as well as some coefficients of the extended matrix Eq. (16)) for the case of coating and substrate being of the same material were obtained in [12]. The results were obtained on the base of solution of the matrix Wiener-Hopf problem [17], which was extended to describe displacements. The extraction of the coefficient a_{22} for this case was made before [18], [19]. 3-D case was considered in [20].

It follows from the results of [5] that the value for a_{12} does not effectively depend on the ratio elastic moduli, unless very soft substrates. For this case value

$$a_{12} = \sqrt{3} \tag{22}$$

was obtained [12]. It was also obtained (ibid.) the value for a_{13} for the case of the same moduli of coating and substrate

$$a_{13} = 1 + \sqrt{3} \tag{23}$$

The obtained formula for a_{11} appeared rather awkward to be represented here.

An intent look at the results for a_{11} reveals that all points may be represented as a single master curve (Fig 3) with rather good accuracy.

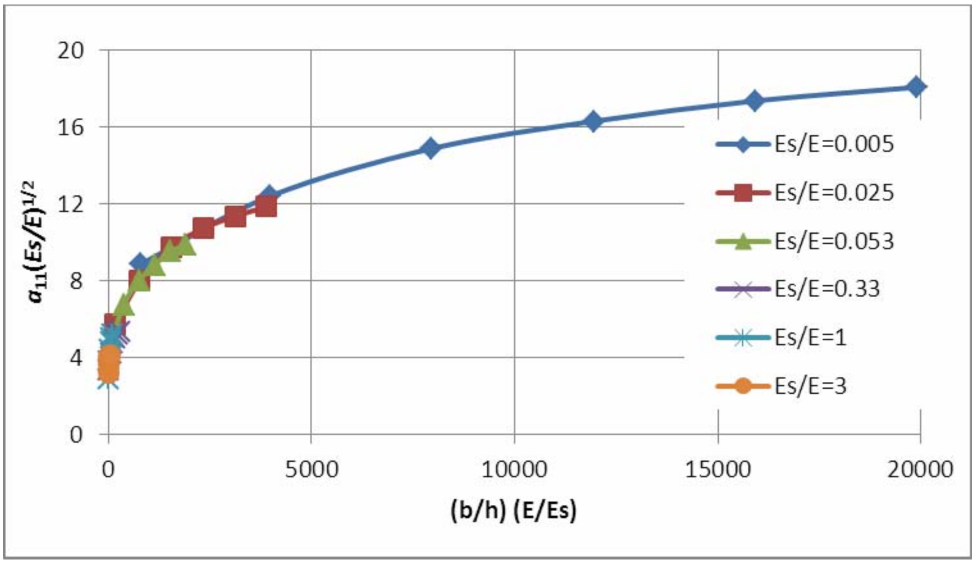

Fig. 3. Numerically obtained master curve for a_{11} on the base of results [5].

The curve may be fitted by one of the following (purely approximating) formulae

$$a_{11} = \frac{1}{2}\sqrt{\frac{E}{E_S}} + \frac{3}{2}\left[\frac{b}{h}\left(\frac{E}{E_S}\right)^3\right]^{1/4} \qquad a_{11} = \frac{3}{2}\left[\frac{b}{h}\left(\frac{E}{E_S}\right)^3\right]^{1/4}$$
$$a_{11} = \sqrt[3]{\frac{E}{E_S}}\left[\left(\frac{b}{h}\frac{E}{E_S}\right)^{1/5} - 1\right] \qquad a_{11} = \sqrt{\frac{E}{E_S}}\left[4\left(\frac{b}{h}\frac{E}{E_S}\right)^{1/6} - 3\right] \tag{24}$$

7. Some asymptotic estimations for critical stress

For γ_σ . slightly diverging from unity, which corresponds to small β, asymptotic solution of Eq. (11) may be obtained by the following substitution

$$\sqrt{\gamma_\sigma} = 1 + a_1\beta^m + a_2\beta^n + ... \tag{25}$$

On expanding Eq. (25) into series for small β, the coefficients a_1, a_2, as well as exponents m, n for which the solution exists are found. The corresponding solution is

$$\sigma^{cr} = \frac{\pi^2 h^2 E^*}{12b^2}\left(1 - 2d_0\beta + 3d_0^2\beta^2 + ...\right) \tag{26}$$

Dependence of γ_σ on β . according to this model is also presented on Fig. 2.

The carried FE analysis [9], the results of which are presented on Figure 2 (dots), confirms the analytically obtained dependence of the critical stress on the elastic and geometric parameters according to the suggested models.

Summary

The problem of a crack propagation in multilayered coating either between the individual layers, or between the whole package forming the coating and substrate (possibly also non-uniform) is considered. According to the model the delaminated part of the coating is treated as a plate with a special attention given to the boundary conditions, which are supposed to be of the elastic clamping type, which means that the angle of rotation at the clamping point is related to the acting bending moment at that point. The generalized model of elastic clamping is also considered in the frame of which it is supposed that components of displacements and angle of rotation at the clamping point are related to the acting total force and total moment by means of 3x3 matrix of elastic coefficients. Several variants of analytical models to determine the coefficients of this 3x3 matrix were considered and discussed. The case of non-uniform (multi-layered) coating is considered with a special attention paid to analysis of the influence of the relative dimensions involved, such as the individual layer and the multilayer coating thicknesses, distance from the crack to the free surface, crack length.

Using the obtained solution the problem on buckling of the delaminated coatings is addressed. It has been shown that the difference between the obtained critical stress and the critical stress of a rigidly clamped plate can be significant. It has also been shown that for a wide range of parameters even for anisotropic and multilayered structures the ratio of the obtained critical stress and the critical stress of a rigidly clamped plate is determined by a single nondimensional parameter, which is a combination of the elastic constants of the coating and substrate, and the ratio of the delamination length to the coating thickness. The analytical results correlate well with the results obtained using the numerical calculations.

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