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Residual Stresses in Thick, Nonhomogeneous Coatings

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Residual macrostresses in thick, nonhomogeneous planar coatings are investigated theoretically using the methods of the isotropic theory of elasticity. The dependence of the elastic properties and of the sources of residual stresses on the coordinate perpendicular to the interface is considered. The results can be applied to thick graded or sandwich coatings. A simplification of the results for the cases of homogeneous and thin coatings is shown. Some differences for coatings on cylindrical and spherical surfaces are also mentioned.

Keywords cylindrical coatings, graded and layered coatings, planar coatings, residual stresses, spherical coatings, thick coatings

1. Introduction

Much attention has been paid to the theory of macroscopic residual stresses in coatings (see, for example, Ref 1-3). Usually a platelike specimen is assumed, made of a homogeneous coating on a homogeneous substrate, each with different physical properties. Approximations are often used for thin films when the thickness of the coating is much smaller than the thickness of the substrate.

Three main theoretical approaches can be distinguished in the literature. In the first, "elementary" approach, the residual stresses are calculated for a known distribution of the sources of residual stresses (changes of temperature, distribution of impurities, etc.) in the final coating/substrate system (Ref 4-7).

In the second, more complex, approach, the gradual formation of the residual stresses during and after the deposition is modeled (Ref 8, 9). In the third, inverse approach, a theoretical analysis is used to evaluate residual stresses from measurements of deformation on the coating/substrate system (Ref 10-13).

Another important problem that has been studied recently is the theoretical analysis of the stress concentrations at the coating edges, cracks in the coatings and in the interface between the coating and substrate, and their relationship to fracture (Ref 14-16).

This paper will concentrate, within the "elementary" approach described, on the theory of macroscopic residual stresses in thick, nonhomogeneous (graded or layered) coatings. The sources of residual stresses (quasi-plastic deformations) will be given as functions of the coordinate perpendicular to the interface, but will not change in the directions parallel to the interface. The analytical solution developed in detail in Ref 17 and 18 will be used for platelike specimens, and differences for cylindrical and spherical specimens (Ref 19, 20) will be mentioned. Special cases and simplifications of the general results for homogeneous coatings and for thin coatings will also be discussed.

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2. Comments on Residual Stresses in Nonhomogeneous Bodies

The sources of residual stresses will be assumed to be given by the tensor of quasi-plastic deformations, $e^0_{ij}(x_m, t)$, due to distribution of impurities, temperature variations and phase changes, or plastic deformation, depending on the coordinates x_m and on time t. However, only slow time changes will be assumed so that the dynamic effects can be neglected and the static theory of elasticity can be used. The development of residual stresses can be studied in this way with t as a scalar parameter.

Nomenclature	
A	constant, m^{-1}
B	constant
e^0_{ij}, e^0	quasi-plastic deformation
e^T_{ij}, e^T	total deformation
e_{ij}, e	elastic deformation
E	Young's modulus, Pa
h	thickness, m
k, K	dimensionless parameters
r	radius, m
R	radius of curvature, m
x, y, z	cartesian coordinates, m
T	temperature, K
u^T_i	total displacements, m
Y	elastic constant, Pa
Greek symbols	
α	coefficient of thermal expansion, K^{-1}
υ	Poisson's ratio
σ_{ij}, σ	stress, Pa
ϑ, φ	angles
Subscripts	
0	substrate
1	coating
i	serial number of a layer
f	final

For the final state studied in this paper, the parameter t will be left out.

The quasi-plastic deformation will be supposed small:

$$|e^0_{ij}(x_k)| << 1 \quad \text{(Eq 1)}$$

so that the linear theory of elasticity can be used.

The total deformation, e^T_{ij}, can be written as the sum of quasi-plastic e^0_{ij} and elastic e_{ij} deformations:

$$e^T_{ij} = e^0_{ij} + e_{ij} \quad \text{(Eq 2)}$$

where the total deformation is compatible; that is, total displacements, u^T_m, exist:

$$e^T_{ij} = \frac{1}{2}\left[\left(\frac{\partial u^T_i}{\partial x_j}\right) + \left(\frac{\partial u^T_j}{\partial x_i}\right)\right] \quad \text{(Eq 3)}$$

and e^T_{ij} fulfills the equations of compatibility:

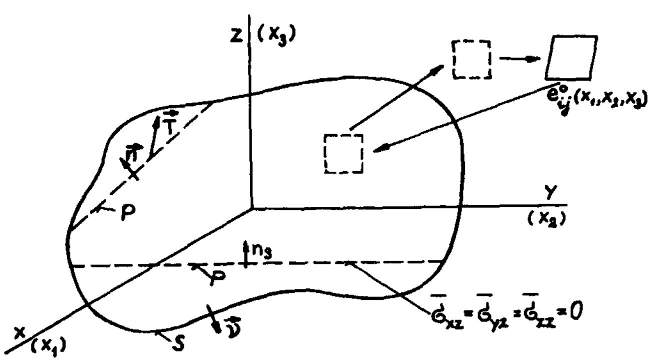

Fig. 1 Nonhomogeneous body with residual stresses due to quasi-plastic deformations $e^0_{ij}(x_1, x_2, x_3)$

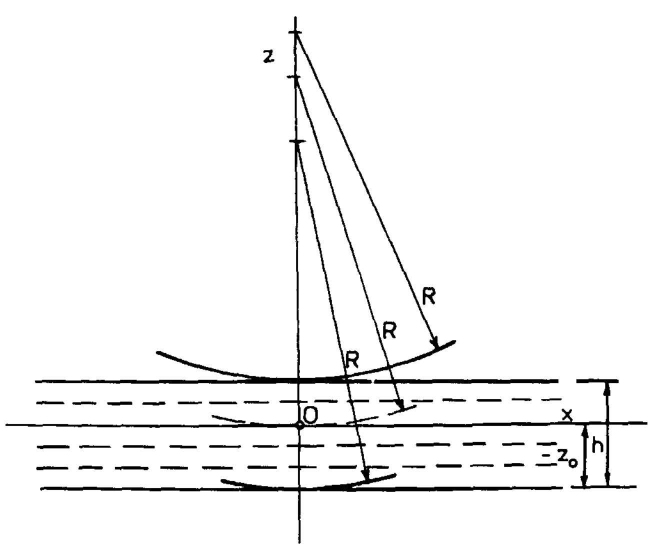

Fig. 2 Bending of the plate due to residual stresses

$$\frac{\varepsilon_{ijk}\,\varepsilon_{lmn}\,\partial^2 e^T_{jn}}{\partial x_k\,\partial x_m} = 0 \quad \text{(Eq 3a)}$$

where ε_{ijk} is the Levi-Civita antisymmetric tensor and Einstein's summation convention is used (Ref 21).

In the elastically nonhomogeneous, generally anisotropic continuum with elastic stiffness coefficients $C_{ijkl}(x_m)$, the residual stresses σ_{ij} follow from Hooke's law:

$$\sigma_{ij} = C_{ijkl}\, e_{kl} \quad \text{(Eq 4)}$$

where $e_{kl} = e^T_{kl} - e^0_{kl}$ are the elastic deformations. The stresses must fulfill the equilibrium conditions (with zero volume forces):

$$\frac{\partial \sigma_{ij}}{\partial x_i} = 0 \quad \text{(Eq 5)}$$

and the boundary conditions of zero external tractions:

$$\nu_i \sigma_{ij} = 0 \quad \text{(Eq 6)}$$

at points $x^{(S)}_m$ of the body surface S with normals $\nu_i(x^{(S)}_m)$ (Fig. 1).

Equations 1 to 6 are written in the same form as for homogeneous bodies. Their solution for homogeneous isotropic bodies is discussed in detail in Ref 22. However, their solution for nonhomogeneous bodies is much more complicated because of the dependence of C_{ijkl} on the local coordinate. For example, the three equations for total displacements, u^T_m, after substitution of Eq 2 to 4 into Eq 5,

$$\frac{\partial}{\partial x_i}\left\{C_{ijkl}(x_m)\left[\frac{1}{2}\left[\left(\frac{\partial u^T_k}{\partial x_l}\right) + \left(\frac{\partial u^T_l}{\partial x_k}\right)\right] - e^0_{kl}(x_m)\right]\right\} = 0 \quad \text{(Eq 7)}$$

are three differential equations ($j = 1, 2, 3$) of the second order for u^T_m. These equations, however, have variable coefficients, $\partial C_{ijkl}/\partial x_i$ and C_{ijkl}, and can be solved analytically only in special cases.

Up to now we have assumed that e^0_{ij} and C_{ijkl} are continuous functions of x_m with continuous derivatives. The solution simplifies for a nonhomogeneous body composed of n elastically homogeneous regions. Inside each region, $r = 1, 2, \ldots, n$, the stiffnesses $C^{(r)}_{ijkl}$ are constant, and hence Eq 7 simplifies. However, the solutions for individual regions, $u^{T(r)}_m$ and $\sigma^{(r)}_{ij}$, must satisfy the interface conditions. For the so-called well-bonded interface, displacements u^T_m and tractions $T_j = \nu_i\sigma_{ij}$ must cross the interfaces continuously.

Two simple, useful theorems on average residual stresses are a direct consequence of zero external forces:

- The average values, $\overline{T}_j$, of tractions $T_j = n_i\sigma_{ij}$ over any plane P with normal n_i are zero. For example, for planes parallel to the xy plane,

$$\overline{\sigma}_{zz} = (1/P)\iint_P \sigma_{zz}\, dx\, dy = 0$$

and in a similar way, $\overline{\sigma}_{xz} = \overline{\sigma}_{yz} = 0$.

- The average values, $\bar{\bar{\sigma}}_{ij}$, of the residual stress components σ_{ij} in Cartesian coordinates over the whole volume V of the body are zero. It can be shown for $\bar{\bar{\sigma}}_{zz}$ by integration of $\bar{\sigma}_{zz}$ over z,

$$\bar{\bar{\sigma}}_{zz} = \left(\frac{1}{V}\right)\iiint_V \sigma_{zz}\, dx\, dy\, dz = 0$$

These theorems are general. They are valid for homogeneous and nonhomogeneous, isotropic and anisotropic bodies and even hold for large deformations.

The solution of the system of Eq 1 to 6 simplifies substantially for coatings with some special symmetries, as described in the following sections.

3. Nonhomogeneous Planar Coatings

3.1 *General Solution for Residual Stresses*

A plate infinite along the xy plane and of thickness h in the z direction is considered (Fig. 2), with Young's modulus, E, and Poisson's ratio, ν, being (continuous or discontinuous) functions of coordinate z perpendicular to the plate plane:

$$E = E(z)$$

$$\nu = \nu(z)$$

$$z_0 \leqq z \leqq z_0 + h \qquad \text{(Eq 8)}$$

That is, the plate is locally isotropic, but nonhomogeneous in the z direction.

The sources of residual stresses are given by quasi-plastic deformations:

$$e^0_{xx} = e^0_{yy} = e^0(z)$$

$$e^0_{zz} = e_z(z)$$

$$e^0_{xy} = e^0_{xz} = e^0_{yz} = 0 \qquad \text{(Eq 9)}$$

which are isotropic and homogeneous in the xy planes. No external forces act at the plate surfaces and at infinity.

Because of the symmetry of the problem, the solution cannot depend on x and y and only two stress components are nonzero:

$$\sigma_{xx}(z) = \sigma_{yy}(z) = \sigma(z)$$

$$\sigma_{zz} = 0$$

$$\sigma_{xy} = \sigma_{xz} = \sigma_{yz} = 0 \qquad \text{(Eq 10)}$$

Furthermore,

$$e^{\mathrm{T}}_{xx} = e^{\mathrm{T}}_{yy} = e^{\mathrm{T}}(z)$$

$$e^{\mathrm{T}}_{zz} = e^{\mathrm{T}}_z(z)$$

$$e^{\mathrm{T}}_{xy} = e^{\mathrm{T}}_{xz} = e^{\mathrm{T}}_{yz} = 0$$

$$e_{xx} = e_{yy} = e(z)$$

$$e_{zz} = e_z(z)$$

$$e_{xy} = e_{xz} = e_{yz} = 0$$

(Eq 11)

Also, Hooke's law can be written in the form:

$$e = e^{\mathrm{T}} - e^0 = \frac{1-\nu}{E}\sigma$$

$$e_z = e^{\mathrm{T}}_z - e^0_z = -\frac{2\nu}{E}\sigma \qquad \text{(Eq 12)}$$

where all the quantities are functions of z.

The tensor of total deformation, e^{T}_{ij}, must fulfill the compatibility equations (Eq 3a), which simplify in our case to one equation, $d^2e^{\mathrm{T}}/dz^2 = 0$, with the solution:

$$e^{\mathrm{T}} = \mathrm{A}z + \mathrm{B} \qquad \text{(Eq 13)}$$

where A and B are constants.

The nonzero stress component, σ, then follows from Hooke's law as:

$$\sigma(z) = Y(z)[\mathrm{A}z + \mathrm{B} - e^0(z)] \qquad \text{(Eq 14)}$$

where the appropriate local elastic constant is:

$$Y(z) = \frac{E(z)}{1-\nu(z)} \qquad \text{(Eq 15)}$$

The stresses already meet equilibrium equations (Eq 5) and boundary conditions (Eq 6) at the plate surfaces: $z = z_0$ and $z = z_0 + h$.

The constants A and B can be determined from the condition of zero forces and moments at infinity:

$$\int_{z_0}^{z_0+h} \sigma(z)\, dz = 0$$

$$\int_{z_0}^{z_0+h} \sigma(z)\, z\, dz = 0 \qquad \text{(Eq 16)}$$

When Eq 14 is inserted in Eq 16, a system of two linear algebraic equations for the constants A and B follows:

$$\mathrm{SA} + \mathrm{FB} = \mathrm{N}$$

$$\mathrm{IA} + \mathrm{SB} = \mathrm{M} \qquad \text{(Eq 17)}$$

where the constants F, S, I, N, and M are given in the form of integrals:

$$F = \int_{z_0}^{z_0+h} Y\,dz$$

$$S = \int_{z_0}^{z_0+h} Y z\,dz$$

$$I = \int_{z_0}^{z_0+h} Y z^2\,dz$$

$$N = \int_{z_0}^{z_0+h} Y e^0\,dz$$

$$M = \int_{z_0}^{z_0+h} Y e^0 z\,dz \qquad \text{(Eq 18)}$$

Therefore, the constants A and B can be calculated as:

$$A = \frac{(FM - SN)}{(FI - S^2)}$$

$$B = \frac{(IN - SM)}{(FI - S^2)} \qquad \text{(Eq 19)}$$

where

$$D = (FI - S^2) > 0$$

The stresses in the plate are now determined: There are tensile or compressive stresses $\sigma(z)$ parallel to the plate surface (isotropic; i.e., the same in all directions in the xy plane) with the dependence on z given by Eq 14, where the constants A and B are given by Eq 19 with Eq 18. The stresses depend on quasi-plastic deformation $e^0(z)$, but not on $e_z^0(z)$; there is a free dilatation in the z direction.

The total deformations $e^T(z)$ and $e_z^T(z)$ follow from Eq 13 and 12 with Eq 14, and the total displacements u_i^T can be calculated from Eq 3 as:

$$u_x^T = Azx + Bx$$

$$u_y^T = Azy + By$$

$$u_z^T = -\left(\frac{A}{2}\right)(x^2 + y^2) + \int_0^z e_z^T(z)\,dz \qquad \text{(Eq 20)}$$

The displacements in the vicinity of an arbitrarily chosen point, $x = y = 0$, are given as functions of x, y, and z. The system of planes z = const. will be deformed into a system of rotational parabolic surfaces with the radius of curvature R at the point $x = y = 0$:

$$R = -\left(\frac{1}{A}\right) \qquad \text{(Eq 21)}$$

where A is given by Eq 19. For A > 0 ($R < 0$), the center of curvature is in the lower half-space and for A < 0 ($R > 0$) in the upper half-space (Fig. 2).

3.2 *Comment on Plane Strain and Plane Stress*

A plate that is infinite in dimension in the xy plane and with zero forces at infinity has been considered thus far. This state can be called the "free plate" state. Some authors consider a different mode of the plate deformation:

- For plane strain with respect to xz planes, the condition $e_{yy}^T = 0$ is introduced and the symmetry condition $\sigma_{xx} = \sigma_{yy}$ is then no longer valid. Instead, $\sigma_{yy} = \nu\sigma_{xx} - e^0E$, and Hooke's law takes the form:

$$e_{xx} = \left(\frac{1-\nu^2}{E}\right)\sigma_{xx} + \nu e^0$$

$$e_{yy} = -e^0$$

$$e_z = -\left[\frac{\nu(1-\nu)}{E}\right]\sigma_{xx} + \nu e^0 \qquad \text{(Eq 12a)}$$

  The solution is completely given by $\sigma_{xx}(z) = \sigma(z)$, which can again be calculated from Eq 14 with Eq 17 to 19, with the following modification: Now $Y = E/(1 - \nu^2)$ and $(1 + \nu)e^0$ appears instead of e^0 in Eq 14. Note that the stresses are no longer purely residual, as external forces have to act at external xz planes.

- For plane stress with respect to xz planes—that is, for a thin band in the y direction (and infinite only in the x direction)—$\sigma_{yy} = 0$ and Hooke's law simplifies to:

$$e_{xx} = \left(\frac{1}{E}\right)\sigma_{xx}$$

$$e_{yy} = e_z = -\left(\frac{\nu}{E}\right)\sigma_{xx} \qquad \text{(Eq 12b)}$$

  The solution is again completely given by $\sigma_{xx}(z) = \sigma(z)$, which can be calculated from Eq 14 with Eq 17 to 19, with one modification: $Y = E$.

In further considerations, the "free plate" state defined by Eq 9 to 12 will be assumed. The cases of plane strain and plane stress can be treated with trivial modifications. The stress component $\sigma_{xx} = \sigma(z)$ follows from Eq 14 with the mentioned changes; however, the expressions for u_i^T differ slightly from Eq 20, but Eq 21 for curvature remains valid in the xz plane.

3.3 *Comment on Similarity*

An additional comment from the point of view of similarity in nonhomogeneous elastic bodies can be proved if nondimensional coordinates $x' = x/h$, $y' = y/h$, and $z' = z/h$ are introduced.

In plates of different thickness h with the same dependences of the elastic constants $E(z')$ and $\nu(z')$ and of quasi-plastic deformation $e^0(z')$ on z' (i.e., in "similar" plates), the stresses $\sigma_{ij}(z')$

and the deformations $e_{ij}^{T}(z')$ and $e_{ij}(z')$ at the corresponding points $z' = z/h$ are identical. They do not depend on h.

On the other hand, the displacements u_x^T, u_y^T, and u_z^T, as well as the radius of curvature R, are linearly proportional to h.

3.4 *Residual Stresses in a Nonhomogeneous Coating with a Linear Dependence of Properties on z*

For a homogeneous substrate of thickness h_0, the origin of coordinates will be chosen at the interface, that is, $z_0 = -h_0$ (Fig. 3a). Then in the substrate, $-h_0 \leqq z < 0$, the elastic constant, $Y = Y_0 = E_0/(1 - \nu_0)$, and the linear thermal expansion coefficient, $\alpha = \alpha_0$, are constant.

The coating of thickness h_1 varies in its properties Y and α linearly from the values Y_0 and α_0 in the interface to the given values Y_1 and α_1 at the upper surface; for $0 < z \leqq h_1$, $Y = Y_0 + (Y_1 - Y_0)(z/h_1)$ and $\alpha = \alpha_0 + (\alpha_1 - \alpha_0)(z/h_1)$. Residual thermal stresses are due to cooling of the entire plate from T to T_f so that in the substrate $e_0^0 = \alpha_0(T_f - T)$ is constant and in the coating, for $0 < z \leqq h_1$:

$$e^0 = [\alpha_0 + (\alpha_1 - \alpha_0)(z/h_1)](T_f - T)$$

$$= e_0^0 + (e_1^0 - e_0^0)(z/h_1)$$

In this case, the constants F, S, I, N, and M can be calculated by integration from Eq 18 and are given in detail in Ref 17.

The results will be illustrated for a special case. Here, the substrate is of steel ($Y_0 = 285$ GPa, $\alpha_0 = 12 \times 10^{-6}$ K^{-1}) and the properties of the coating vary linearly from these values at the interface to the values of alumina at the upper surface ($Y_1 = 450$ GPa and $\alpha_1 = 8 \times 10^{-6}$ K^{-1}). Residual stresses have developed during cooling from $T = 1020$ °C to $T_f = 20$ °C, so that $e_0^0 = -12 \times 10^{-3}$ and $e_1^0 = -8 \times 10^{-3}$. The ratio of the coating and substrate thickness is chosen to be $h_1/h_0 = 1/10$. The residual stresses $\sigma(z)$ in a plate from Fig. 3(a) are given in Fig. 4 by solid lines. Because of a continuous course of $Y(z)$ and $e^0(z)$, $\sigma(z)$ is also continuous at the interface. The radius of curvature is $R/h_1 = -8.42 \times 10^3$. In a plate with two-sided symmetrical coatings (Fig. 3b), the stresses are given in Fig. 4 by a dashed line.

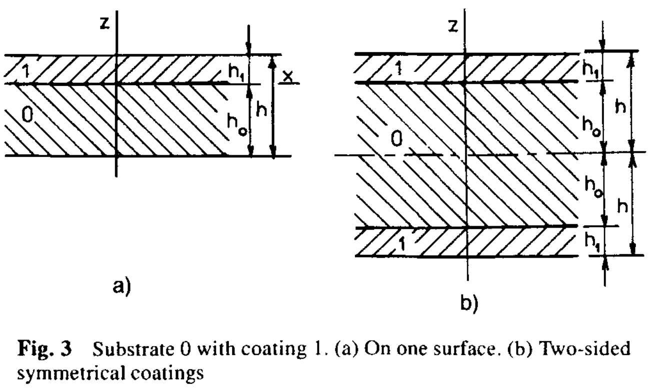

Fig. 3 Substrate 0 with coating 1. (a) On one surface. (b) Two-sided symmetrical coatings

3.5 *Lamellar Coatings*

For a plate composed of $n + 1$ homogeneous layers of thickness $h_i = z_{i+1} - z_i$, where $i = 0, 1, 2, \ldots, n$ (in other words, a substrate of thickness h_0 covered by n homogeneous coatings), the elastic constants E_i and ν_i, and thus also $Y_i = E_i/(1 - \nu_i)$, are constant within each layer. The quasi-plastic deformation e_i^0 will also be taken constant in each layer; in the case of residual thermal stresses due to cooling from high temperature T to the final temperature T_f, it is $e_i^0 = \alpha_i(T_f - T)$, with constant α_i, T_f, and T.

Integrals in Eq 18 can be calculated as:

$$F = \sum_{i=0}^{n} Y_i h_i$$

$$S = \left(\frac{1}{2}\right) \sum_{i=0}^{n} Y_i (z_{i+1}^2 - z_i^2)$$

$$I = \left(\frac{1}{3}\right) \sum_{i=0}^{n} Y_i (z_{i+1}^3 - z_i^3)$$

$$N = \sum_{i=0}^{n} e_i^0 Y_i h_i$$

$$M = \left(\frac{1}{2}\right) \sum_{i=0}^{n} e_i^0 Y_i (z_{i+1}^2 - z_i^2) \qquad \text{(Eq 22)}$$

The constants A and B then follow directly from Eq 19. The stresses $\sigma(z)$ can be obtained from Eq 14:

$$\sigma_k(z) = Y_k(Az + B - e_k^0)$$

$$z_k < z < z_{k+1} \qquad \text{(Eq 23)}$$

For discontinuous changes of $Y(z)$ and $e^0(z)$, the stresses $\sigma(z)$, elastic deformations $e(z)$ and $e_z(z)$, and total deformation $e_z^T(z)$ will also be discontinuous at the interfaces $z = z_1, z_2, \ldots, z_n$. On the other hand, the total deformation $e^T(z) = Az + B$ and the total

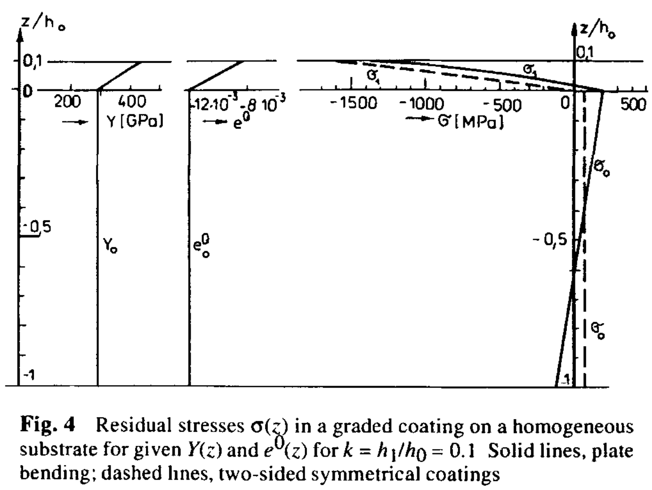

Fig. 4 Residual stresses $\sigma(z)$ in a graded coating on a homogeneous substrate for given $Y(z)$ and $e^0(z)$ for $k = h_1/h_0 = 0.1$ Solid lines, plate bending; dashed lines, two-sided symmetrical coatings

displacements u_x^T, u_y^T, and u_z^T given by Eq 20 remain continuous functions of z. The radius of curvature remains according to Eq 21, $R = -1/A$.

In cases when the plate does not bend—for example, for a symmetrical arrangement with respect to the central plane (similarly as in Fig. 3b for $n = 1$)—$A = 0$ and the stresses are then constant in each layer:

$$\sigma_k = Y_k \frac{\left[\sum_{i=0}^{n} (e_i^0 - e_k^0)\, Y_i h_i\right]}{\left[\sum_{i=0}^{n} Y_i h_i\right]} \quad \text{(Eq 24)}$$

Lamellar coatings have been treated in a similar way in Ref 23.

3.6 *Simplification for a Homogeneous Coating*

3.6.1 Thick Coating

For a plate made of a homogeneous coating of thickness h_1 on a homogeneous substrate of thickness h_0, the elastic parameters $Y_1 = E_1/(1 - \nu_1)$ and $Y_0 = E_0/(1 - \nu_0)$ are constant. The quasi-plastic deformations e_1^0 (e.g., $e_1^0 = \alpha_1(T_f - T_1)$) and e_0^0 (e.g., $e_0^0 = \alpha_0(T_f - T_0)$) will also be assumed to be constant. We shall give the exact solution for this case, in contrast to the simplified formulas that are only approximately valid for very thin coatings, often used in the literature. The solution follows as a special case of lamellar coatings for $n = 1$ from Eq 23, 22, and 19.

It can be shown by rearrangement of the expressions $(B - e_1^0)$ and $(B - e_0^0)$ in Eq 23 that the stresses are proportional to the difference of dilatations $(e_1^0 - e_0^0)$:

$$\sigma_1(z) = Y_1(e_1^0 - e_0^0)\frac{[c(z/h_0) - b_1]}{d} \text{ for } 0 < z \leqq h_1$$

$$\sigma_0(z) = Y_0(e_1^0 - e_0^0)\frac{[c(z/h_0) + b_0]}{d} \text{ for } -h_0 \leqq z < 0 \quad \text{(Eq 25)}$$

where

$$c = 6K(k + k^2)$$

$$b_1 = 1 + K(3k^2 + 4k^3)$$

$$b_0 = K(4k + 3k^2) + K^2k^4$$

$$d = 1 + K(4k + 6k^2 + 4k^3) + K^2k^4 \quad \text{(Eq 26)}$$

Here, the nondimensional parameters k and K are used:

$$k = \frac{h_1}{h_0}$$

$$K = \frac{Y_1}{Y_0} \quad \text{(Eq 27)}$$

The radius of curvature $R = -1/A$ can be written in the form:

$$R = -\frac{dh_0}{6K(e_1^0 - e_0^0)(k + k^2)} \quad \text{(Eq 28)}$$

The stresses are discontinuous and of opposite sign at the interface $z = 0$: $\sigma_1(0^+) = -Y_1(e_1^0 - e_0^0)b_1/d$, $\sigma_0(0^-) = Y_0(e_1^0 - e_0^0)b_0/d$. The stresses reach zero values at points $z_1' = b_1h_0/c$ and $z_0' = -b_0h_0/c$ if $z_1' < h_1$ and $z_0' > -h_0$. This solution is equivalent to that given previously by Chiu (Ref 24), which is presented in a different form and derived in a different way.

The results simplify when bending is prevented, for example, for two-sided symmetrical coatings (Fig. 3b). It follows directly from Eq 24 with $n = 1$ that the stresses are then constant in the coating and in the substrate:

$$\sigma_1 = \frac{Y_1(e_0^0 - e_1^0)}{(1 + Kk)}$$

$$\sigma_0 = \frac{Y_0(e_1^0 - e_0^0)Kk}{(1 + Kk)} = \frac{Y_1(e_1^0 - e_0^0)k}{(1 + kK)} \quad \text{(Eq 29)}$$

where, of course, $\sigma_0 = -k\sigma_1$.

The stresses given in Eq 25 and 29 are compared in Fig. 5 for a special case of a homogeneous alumina coating on a steel substrate with the numerical values of all parameters given in section 3.5 ($k = 0.1$, $K = 1.591$, $Y_1(e_1^0 - e_0^0) = 1818$MPa). It should be mentioned that the value of $Y \approx 450$ GPa corresponds to bulk alumina with low porosity and that for a plasma-sprayed alumina coating the value of Y_1 will be much smaller (because of a smaller value of E_1 due to porosity and the imperfect contact between the deposited splats of material) (Ref 25).

The effect of the thickness ratio $k = h_1/h_0$ on the distribution of stresses for the case of homogeneous coatings (Eq 25 and 29), is illustrated in Fig. 6. The maximum possible stress in the coating for $k \to 0$ is called the saturation stress, $\sigma_{1M} = Y_1(e_0^0 - e_1^0)$.

3.6.2 Simplification for Thin Coatings

The results simplify for a thin coating on a thick substrate, that is, for $k = h_1/h_0 << 1$. They will be introduced under the assumption that the elastic constants Y_1 and Y_0 are of the same order of magnitude—in other words, that the ratio $K = Y_1/Y_0$ is of the order of 1. (The simplification of the results for cases where $K << 1$ or $K >> 1$ can be easily shown in a similar way.) If the members of the order of k^2 are neglected with respect to 1, it follows from Eq 25 and 28 that:

$$\sigma_1 \approx -Y_1(e_1^0 - e_0^0)/(1 + 4kK) \text{ for } 0 < z \leqq h_1$$

$$\sigma_0(z) \approx Y_0(e_1^0 - e_0^0)kK\frac{[6(1 + k)(z/h_0) + (4 + 3k)]}{(1 + 4kK)}$$

$$\text{for } -h_0 \leqq z < 0 \quad \text{(Eq 25a)}$$

with constant stress σ_1 in the coating, however, with bending of the specimen with the radius of curvature $R = -1/A$:

$$R \approx -\frac{h_0(1 + 4kK)}{6kK(e_1^0 - e_0^0)(1 + k)} \quad \text{(Eq 28a)}$$

If the terms of the order of k also are neglected with respect to unity, then:

$$\sigma_1 \approx -Y_1(e_1^0 - e_0^0)$$

$$\sigma_0(z) \approx 4Y_0(e_1^0 - e_0^0)\, kK\left[1 + \left(\frac{3}{2}\right)\left(\frac{z}{h_0}\right)\right]$$

$$\text{for } -h_0 \leqq z < 0 \qquad \text{(Eq 25b)}$$

and with bending:

$$R \approx \frac{h_0}{6kK(e_1^0 - e_0^0)} = \frac{h_0^2 Y_0}{6h_1\sigma_1} \qquad \text{(Eq 28b)}$$

The stresses (Eq 29) in a plate without bending simplify for $k = h_1/h_0 << 1$ to:

$$\sigma_1 \approx -Y_1(e_1^0 - e_0^0)$$

$$\sigma_0 \approx Y_0(e_1^0 - e_0^0)\, kK = Y_1(e_1^0 - e_0^0)(h_1/h_0) \qquad \text{(Eq 29a)}$$

3.7 *Comparison of Nonhomogeneous and Homogeneous Coatings*

The results for graded coatings (section 3.4 and Fig. 4) will now be compared with those obtained for the case of homogeneous coatings (section 3.6 and Fig. 5). Whereas for a graded coating (with a continuous change of elastic and thermal properties across the interface) the stresses at the interface remain relatively small, the stresses in the homogeneous coating at the interface are high. This shows the main advantage of graded coatings: The absolute value of nominal stresses at the interface is smaller; therefore, the concentration of these stresses at interface defects (e.g., at cracks or at coating edges) will also be smaller than in the case of discontinuous changes of properties at the interface. This effect should result in better adhesion of graded coatings.

The thickness dependence of the residual stresses in the coatings from Fig. 6 shows that the stresses are higher in thinner coatings and approach the maximum possible value $\sigma_1 = -Y_1(e_1^0 - e_0^0)$ for $k = h_1/h_0 \to 0$. For thicker coatings, relaxation of the coating stress due to bending and elongation or contraction of the substrate takes place.

This is, of course, valid only under the assumption that the quasi-plastic deformations e_1^0 and e_0^0 do not depend on the coating thickness. However, for some technologies—for example, plasma spraying of coatings—the temperature distribution depends on the thermal conductivity of the coating, the deposition rate, the coating thickness, and other parameters. The quasi-plastic deformations $e_1^0(z)$ and $e_0^0(z)$ then also depend on the coating thickness and may lead on the contrary, to an increase of thermal residual stresses with coating thickness. This effect can be explained by a complex approach based on simulation of the process of deposition.

3.8 *Comments on Some Other Problems*

3.8.1 Deposition Stresses

The residual thermal stresses discussed in sections 3.4 to 3.7 can be called secondary cooling stresses. They are formed after

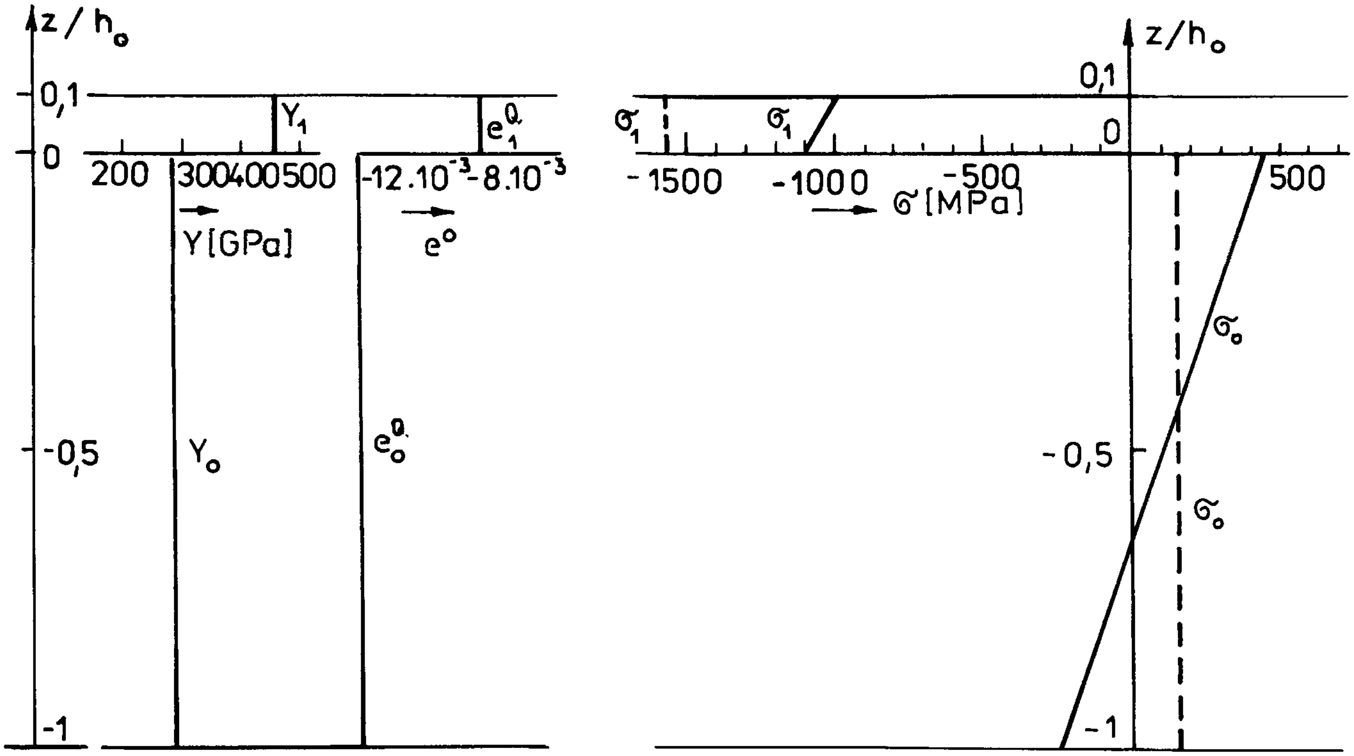

Fig. 5 Residual stresses $\sigma(z)$ in a homogeneous coating on a homogeneous substrate for given Y_1, Y_0 and e_1^0, e_0^0 and for $k = h_1/h_0 = 0.1$. Solid lines, plate bending; dashed lines, two-sided symmetrical coatings

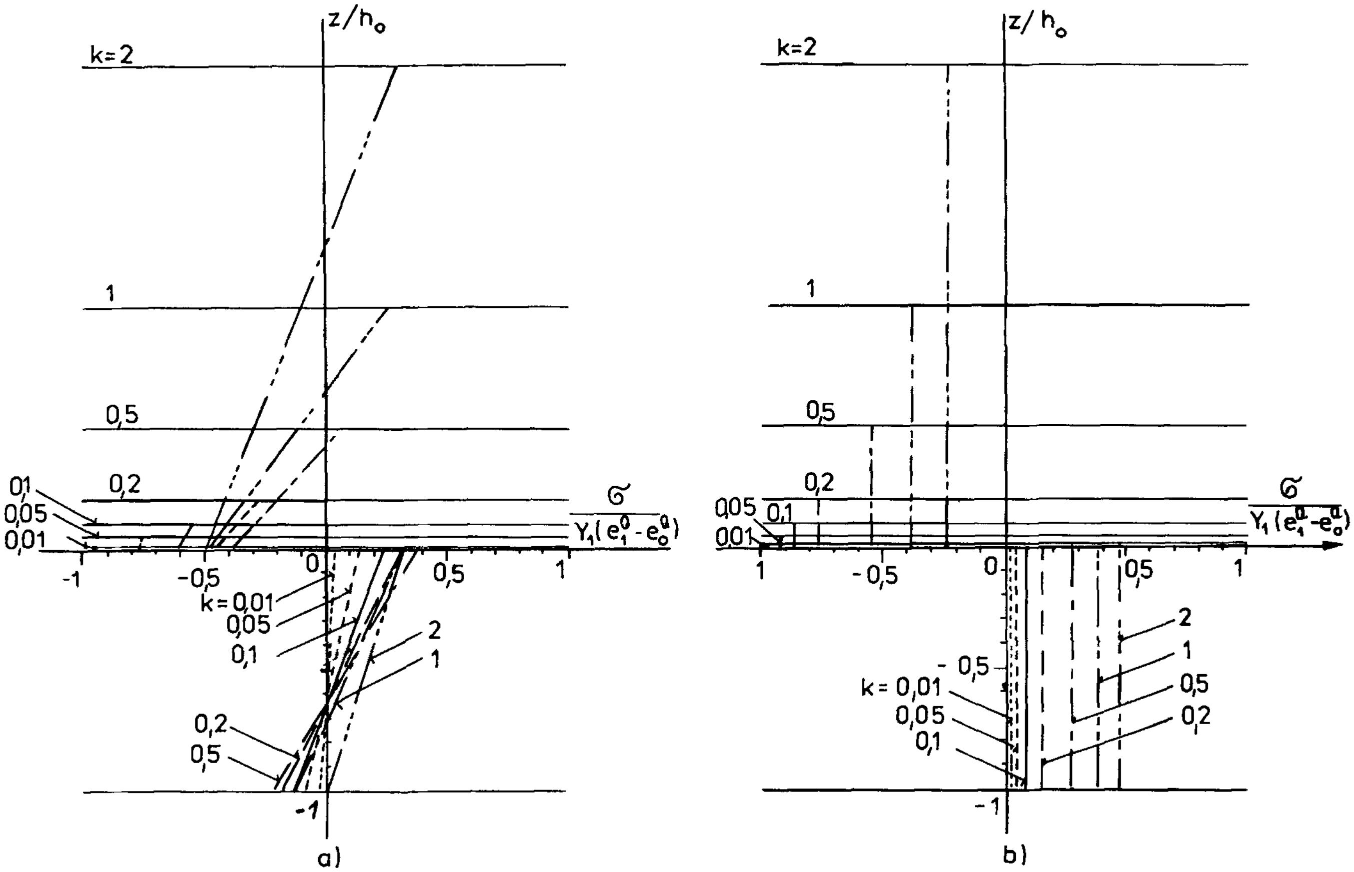

Fig. 6 Effect of the relative coating thickness $k = h_1/h_0$ on stress distribution $\sigma(z)$ in nondimensional units for a homogeneous coating on a homogeneous substrate for $K = Y_1/Y_0 = 1.591$. (a) With bending. (b) For two-sided symmetrical coatings

deposition, during cooling of the entire plate (consisting of the coating and substrate) from high temperature T (or T_1, T_0) to the final temperature T_f.

However, residual stresses can originate during the deposition process itself (e.g., during thermal spraying by gradual deposition of thin layers) as thermal or intrinsic residual stresses. They can be called deposition stresses or, in the case of thermal stresses, primary cooling stresses. During this process, new upper layers influence the stresses in the old lower layers. The formation of the deposition stresses (and also of subsequent secondary cooling stresses) is usually studied within the complex approach by computer simulation (Ref 8, 9).

We have studied (Ref 18) the gradual formation of the primary cooling stresses analytically by a generalization of the approach used in section 3.1. For simplicity, however, the study was conducted for a symmetrical two-sided coating formation (i.e., without bending).

Only one simple example will be mentioned here. The substrate of half-thickness h_0 is held at constant temperature T_f during coating deposition. The homogeneous coatings are gradually and symmetrically deposited as thin layers (of thickness dz), which are cooled from temperature T to T_f before the next thin layer is formed. According to Eq 25b, stress $\sigma_1(z) = -Y_1 e_1^0$, where $e_1^0 = \alpha_1(T_f - T)$ is reached temporarily in the formed thin layer. Figure 7 shows the final deposition stress $\sigma_d(z)$ in the formed coating for different thickness ratios, $k = h_1/h_0$. The stresses reach the maximum tensile value $\sigma_d = -Y_1 e_1^0$ (it is $e_1^0 < 0$) at the upper surface independently of the thickness ratio k; however, they are relaxed inside the coating. On the other hand, the secondary cooling stresses formed by cooling of the final coating/substrate system from T to T_f (section 3.6.1 and Fig. 6b) are compressive in the coating.

3.8.2 Effect of the Substrate Temperature

In sections 3.4 and 3.5, the coating and substrate were assumed to be at the common temperature T at the beginning of the secondary cooling. The effect of the substrate temperature on secondary cooling stresses is illustrated by the following simplified example.

The stresses in the homogeneous coating (with constant $Y_1 = E_1/(1 - \nu_1)$, h_1, α_1) start to form at a high temperature, $T_1 = 1020$ °C. The substrate (with constant $Y_0 = E_0/(1 - \nu_0)$, h_0, α_0) is kept at temperature T_0 (T_1 >= ~T sub 0 ~>= T_f) during deposition, and the entire plate is then cooled to $T_f = 20$ °C.

According to Eq 29a (for $k = h_1/h_0 << 1$), $\sigma_1 = -Y_1(e_1^0 - e_0^0)$, where $e_1^0 = \alpha_1(T_f - T_1)$, $e_0^0 = \alpha_0(T_f - T_0)$, so that the secondary cooling stress in the coating is $\sigma_1 = Y_1[\alpha_1(T_1 - T_f) - \alpha_0 (T_0 - T_f)]$.

The realistic values for the elastic constants of a plasma-sprayed alumina coating are $E_1 \approx 75$ GPa (E_1 is decreased by the effect of microcracks and porosity) and $\nu_1 \approx 0.25$, that is, Y_1

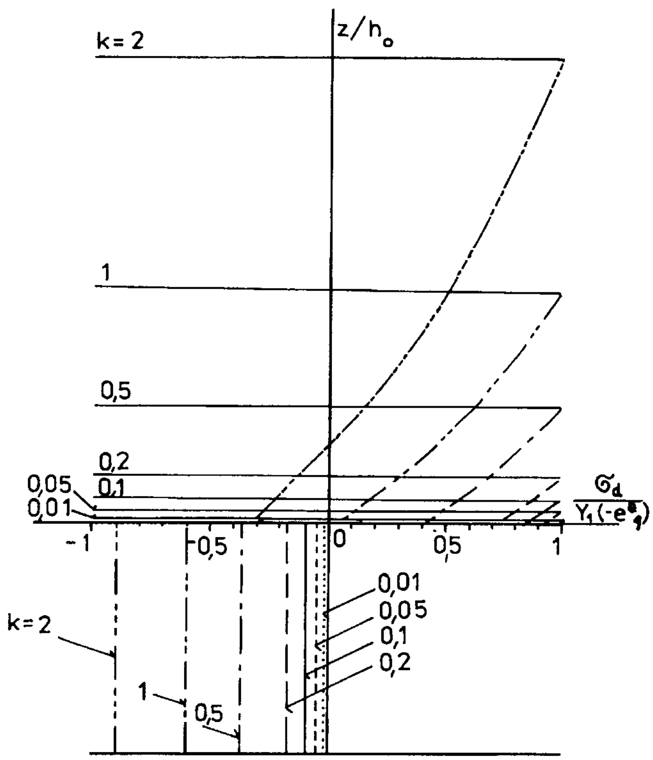

Fig. 7 Effect of thickness ratio $k = h_1/h_0$ on deposition stresses σ_d after fast cooling of new layers during deposition, in alumina coating on steel substrate (K = 1.591, without bending)

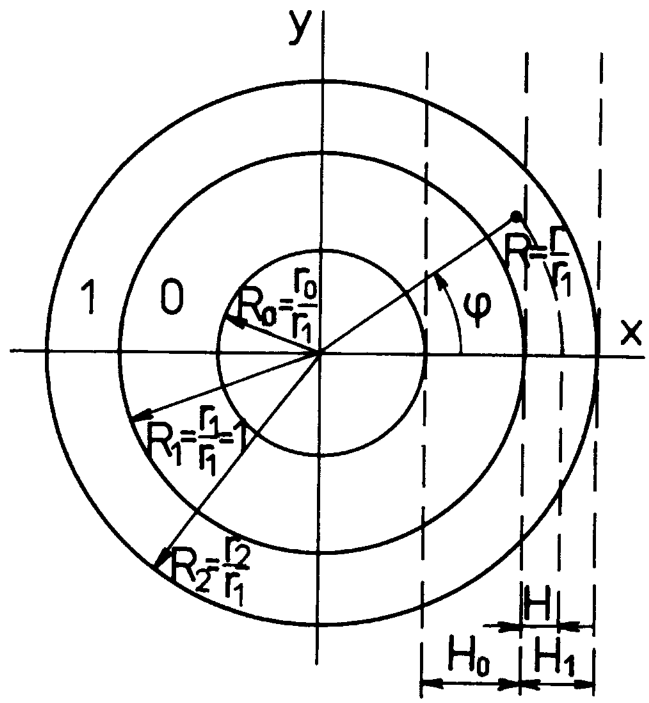

Fig. 8 Substrate tube 0 with coating 1; nondimensional radii $R = r/r_1$ are introduced.

≈100 GPa. Furthermore, $\alpha_1 \approx 8 \times 10^{-6}$ K^{-1}, and for the steel substrate $\alpha_0 \approx 12 \times 10^{-6}$ K^{-1}.

Therefore, for a very hot substrate, $T_0 \approx 1020$ °C, $\sigma_1 \approx -400$ MPa, while for a very cold substrate, $T_0 \approx 20$ °C, $\sigma_1 \approx +800$ MPa. The secondary cooling stress will be zero for $T_0 \approx T_f + (\alpha_1/\alpha_0)(T_1 - T_f)$, that is, for $T_0 \approx 686$ °C. Generally, in thin ceramic coatings on metal substrates (for $\alpha_1 < \alpha_0$), the secondary cooling stresses will be tensile for cold substrates and compressive for hot substrates.

3.8.3 Evaluation of Residual Stresses from Measurements

Equation 28b is usually used for determination of stresses σ_1 in thin coatings (for $h_1 << h_0$) from measurements of curvature after deposition. The evaluation of stress $\sigma_1(z)$ in thick, nonhomogeneous coatings from the measurements of the plate curvature or deformation (based on results of section 3.1) is discussed in Ref 18.

4. Coatings on Cylindrical Surfaces

Residual stresses in thick, nonhomogeneous coatings on cylindrical surfaces have been discussed in Ref 19, where, in cylindrical coordinates r, φ, and z, the quasi-plastic deformations $e_r^0(r)$, $e_\varphi^0(r)$, and $e_z^0(r)$ are assumed to be given as functions of radius r only. In other words, the cylindrical symmetry is preserved. The analysis for thick, nonhomogeneous coatings is more complicated than that for planar coatings (section 3.1).

The results of a special case only will be shown here: a homogeneous, plasma-sprayed alumina coating 1, $r_1 < r < r_2$ (with E_1 = 100 GPa) on a homogeneous steel substrate tube 0, $r_0 < r < r_1$, with given different quasi-plastic volume dilatations, $e_{1r}^0 = e_{1\varphi}^0 = e_{1z}^0 = e_1^0$, $e_{0r}^0 = e_{0\varphi}^0 = e_{0z}^0 = e_0^0$. Nondimensional radii are introduced in Fig. 8, $R = r/r_1$, $R_0 = r_0/r_1$, $R_1 = r_1/r_1 = 1$, $R_2 = r_2/r_1$. The stresses in the substrate and coating, $\sigma_{i\alpha}(r)$ (where i = 0, 1, and $\alpha = r$, φ, z), are given in Fig. 9 in units $\sigma_{1M} = [E_1/(1 - \nu_1)](e_0^0 - e_1^0)$.

For thin coatings, $h_1 = (r_2 - r_1) << h_0 = (r_1 - r_0)$, the results for planar coatings from section 3 can be taken as good approximations for cylindrical coatings, with one modification. There are also nonzero stresses, $\sigma_{0r}(r)$ and $\sigma_{1r}(r)$, in the directions perpendicular to the interface that fulfill the boundary conditions $\sigma_{0r}(r_0) = 0$, $\sigma_{1r}(r_2) = 0$, however, with the value at the interface $\sigma_{0r}(r_1) = \sigma_{1r}(r_1) = -[(r_2 - r_1)/r_1]\sigma_{1M}$. This value, however, is much smaller and of opposite sign than the limiting value of stresses parallel to the interface in thin coatings, $\sigma_{1\varphi} = \sigma_{1z} = \sigma_{1M} = [E_1/(1 - \nu_1)]\,(e_0^0 - e_1^0)$.

5. Coatings on Spherical Surfaces

Residual stresses in thick, nonhomogeneous coatings on spherical surfaces have been discussed in Ref 20, where, in spherical coordinates r, φ, and ϑ, the quasi-plastic deformations $e_r^0(r)$ and $e_\varphi^0(r) = e_\vartheta^0(r)$ are given as functions of radius r only; that is, the spherical symmetry is preserved.

For the special case of a thick, homogeneous alumina coating 1, $r_1 < r < r_2$ (with E_1 = 100 GPa), on a homogeneous substrate in the shape of a full sphere ($r_0 = 0$), $0 < r < r_1$, with different homogeneous quasi-plastic volume dilatations, $e^0_{1r} = e^0_{1\varphi} = e^0_{1\vartheta} = e^0_1$, $e^0_{0r} = e^0_{0\varphi} = e^0_{0\vartheta} = e^0_0$, the stresses in the substrate sphere and in the coating, $\sigma_{i\alpha}(r)$, $i = 0, 1$, $\alpha = r, \varphi, \vartheta$ are given in units $\sigma_{1M} = [E_1/(1 - \nu_1)](e^0_0 - e^0_1)$ in Fig. 10 for three coating thicknesses, with nondimensional radii $R_2 = r_2/r_1 = 2$, 1.1, and 1.01.

For a thin coating on a sphere or a hollow sphere, the results for planar coatings from section 3 can again be taken as good approximations, with one change. There are also nonzero stresses $\sigma_{0r}(r)$ and $\sigma_{1r}(r)$ that fulfill the boundary conditions $\sigma_{0r}(r_0) = 0$ (if $r_0 \neq 0$) and $\sigma_{1r}(r_2) = 0$, however, with the value at the interface $\sigma_{0r}(r_1) = \sigma_{1r}(r_1) = -2[(r_2 - r_1)/r_1]\sigma_{1M}$. This value is again much smaller than the limiting value of stresses in thin coatings parallel to the interface, $\sigma_{1\varphi} = \sigma_{1\vartheta} = \sigma_{1M} = [E_1/(1 - \nu_1)]$ $(e^0_0 - e^0_1)$. However, the value $\sigma_{ir}(r_1)$ for spherical coatings is two times larger than for cylindrical coatings (section 4).

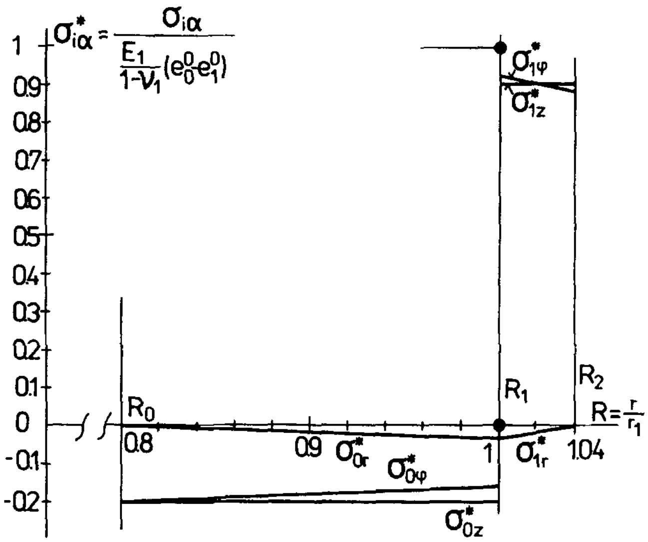

Fig. 9 Residual stresses $\sigma_{i\alpha}$ in units $\sigma_{1M} = [E_1/(1 - \nu_1)](e^0_0 - e^0_1)$ in an alumina coating ($1 < R \leq 1.04$) and a steel tube ($0.8 \leq R < 1$)

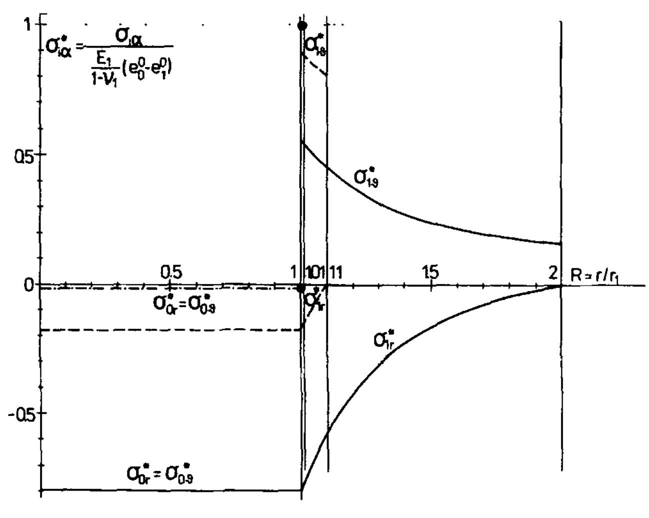

Fig. 10 Residual stresses $\sigma_{i\alpha}$ in units $\sigma_{1M} = \sigma_{1\vartheta\,max} = [E_1/(1 - \nu_1)]$ $(e^0_0 - e^0_1)$ in an alumina coating $1 < R \leq R_2$ on a full steel sphere $0 \leq R < 1$, for three coating thicknesses: $R_2 = 2$, 1.1, and 1.01

6. Discussion

A group of selected problems regarding the theory of residual stresses in coatings has been discussed in this paper. The unifying point is the assumption of thick coatings; that is, the ratio of the coating thickness h_1 to the substrate thickness h_0, $k = h_1/h_0$, can be large. Moreover, the coatings are considered elastically nonhomogeneous, with the elastic properties given by functions of the coordinate z perpendicular to the interface. The general results are then valid for any graded or layered coatings, as well as for nonhomogeneous substrates or for inhomogeneous plates where no distinction need be made between the coating and the substrate.

The sources of residual stresses have been assumed to be given by the quasi-plastic deformations e^0_{ij}. For example, in the case of ion implantation, the quasi-plastic volume dilatation $e^0_{11} = e^0_{22} = e^0_{33} = e^0(z)$ will be proportional to the ion concentration $c(z)$; that is, $e^0 = k_0c(z)$, where $c(z)$ can be taken from measurements or calculated. In the case of secondary cooling stresses, $e^0 = \alpha(z)\ [T_f - T(z)]$, where T_f is the final temperature and $T(z)$ is the temperature at which the stresses start to develop during cooling.

In section 3, a general solution of the residual stresses in planar coatings is given in the so-called elementary approach (for the final coating/substrate system), when the dependence of the elastic constants on z and the distribution of the quasi-plastic deformations $e^0_{ij}(z)$ is known. The solution is given in the analytical form; however, it contains constants given by integrals (Eq 18) which, for complicated dependences $Y(z)$ and $e^0_{ij}(z)$, must be calculated numerically. In the analytically treatable case in section 3.5, for a linear dependence of elastic constants on z in graded coatings, the main advantage of graded coatings is shown: namely, that small residual stresses occur in the interface. Some differences for coatings on cylindrical and spherical surfaces are mentioned briefly in sections 4 and 5.

We have discussed these problems in more detail in Ref 17 to 20. The residual stresses in thick, nonhomogeneous planar coatings have also been studied recently by other authors (Ref 26, 27).

The general results presented may show the limits of application of simple formulas valid for homogeneous and thin coatings.

Some final comments will be made concerning the importance of the residual stresses for fracture in the case of coated systems. Fracture usually starts at defects, especially at microcracks in the coating or in the interface and at the coating edges (Ref 16). An infinite coating (in the x and y directions) with no defects or edges has been considered in this paper, and the resulting residual stresses can be called nominal residual stresses. They can be used as the first step in the theoretical investigation of the fracture process as nominal stresses in the analysis of the crack stability and propagation using fracture mechanics methods. The fracture process is governed by the concentration of the sum of the residual stresses and of the stresses from external loading at the defects, and residual stresses often play the decisive role.

The theory of nominal residual stresses in coatings and its development for nonhomogeneous and thick coatings may be important in terms of improvement of the mechanical properties of bodies with such coatings. It can provide guidelines for the proper choice of materials, of the coating internal structure and thickness, and of the details of the deposition technology (e.g., on heating or cooling of the substrate). This should lead to optimum residual stresses—that is, to small or compressive stresses at the interface or at the upper surface. These results should ensure greater coating lifetimes.

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