Title

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Publication Date

1992-06-01

REPORT NO.
UCB/SEMM-92/15

STRUCTURAL ENGINEERING
MECHANICS AND MATERIALS

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JUNE 1992

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THERMAL STRESSES IN BI-COATED STRUCTURES

By Mauro Ferrari[1] and Luca Lutterotti[2]

ABSTRACT: The thermoelastic problem of a three-phase concentric sphere subject to phase-wise uniform temperature variations is solved exactly. With this solution, the cooldown stresses in a metallic structure with plasma-sprayed oxidation- and thermal-barrier coatings are determined. In this context, the relevance of several control parameters is examined. The general thin-film approximation to the subject problem is presented.

INTRODUCTION

Ceramic coatings have been extensively employed for protection of metallic components subject to thermochemically aggressive environments [Zaat (1983), Miller (1984)]. In its standard implementation, the coating deposition is achieved by plasma-spraying a diffusion (oxidation) barrier first, and subsequently depositing the thermal barrier coating with the same technique. While this method has lead to substantial improvements in the life and efficiency of mechanical components - like combustion chambers and turbine blades - the number of unresolved issues remains considerable [e.g., Zaat (1983), Miller (1984)].

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In particular, thermal stress have been shown to play a central role in the failure modes of coated structures, both under thermal shock conditions or deposition [Miller (1984), Hobbs and Reiter (1988), Bennett (1986), Kvernes and Fartum (1978)], and during service, i.e., when subject to thermal cycling [McDonald and Hendricks (1980), Rickerby et al. (1989)].

In this work, the thermal stress field developed during the cooldown phase of the deposition procedure for a bi-coated spherical body is determined. This goal is achieved by obtaining a closed-form solution for such system subject to phase-wise uniform temperature variations. Thus, two advantages are afforded: (i) The developing of general considerations that apply to bi-coated systems of different nature (e.g., PVD-deposited); and (ii) simplyfying of the analysis of the relevance of various control parameters, which is fundamental for optimal process and material design. In the following developments, attention is focused on the substrate deposition temperature, on the thermoelastic properties of both coating layers, and on the thickness of the coatings. All of these parameters have been considered in experimental investigations [Hobbs and Reiter (1988), Perry et al. (1990), Rickerby et al. (1989)].

The spherical geometry, here employed, permits the exact solutions, and models the state of in-plane elastic constraint and free normal expansion, which is experienced by actual coatings. Uniformly heated, bi-coated structures with non-spherical geometries have been examined by several authors [e. g. Benveniste et al. (1989), Suhir (1988)], employing various approximate methods.

In this work, the thermoelastic properties have been considered as constants for each phase, and their values have been taken from experimental reports. Thus, no effort has been made to relate the microstructure to the macroscopic response. Methods relevant to this problem are presented in Ferrari and Harding (1991) and Ferrari et al. (1991), where the spatial inhomogeneity of the microstructure and the temperature variation are also taken into account.

In the present investigation, the structure is assumed to be stress-free at the instant of termination of the spraying. This is endorsed by the experimental observation of Schmauder and Schubert (1986), but in contrast with the modelling of Takeuchi et al. (1990). Dynamical effects are neglected, as these appear to be relevant in the deposition phase only- see the approximate strain computation scheme of Elsing et al. (1990).

No inelastic processes were here considered. The occurrence of high-temperature superplasticity, viscous flow, and shrinkage cracking, has been reported in the literature [Duclos and Crampon (1987), Schmauder and Schubert (1986)]. The relevance of these mechanisms is presently under investigation.

THE THERMOELASTIC PROBLEM

Generalities

Let the region B+δB, of boundary δB, be occupied by a material of stiffness tensor $\underline{C}$, and be subject to a thermal strain field $\underline{\varepsilon}^*$:

$$\underline{\varepsilon}^* = \underline{\alpha}\, \delta T \qquad (1)$$

where $\underline{\alpha}$ is the thermal expansion tensor, and δT is the temperature variation field. The material properties $\underline{C}$ and $\underline{\alpha}$ are allowed to vary smoothly with position. The strain $\underline{\varepsilon}$, related to the displacement $\underline{u}$ by

$$\underline{\varepsilon} = \text{sym}(\text{grad}(\underline{u})), \quad \text{or} \quad \varepsilon_{ij} = \frac{u_{i,j} + u_{j,i}}{2} \qquad (2)$$

is the sum of the thermal and the mechanical components:

$$\underline{\varepsilon} = \underline{\varepsilon}^* + \underline{e} \tag{3}$$

In thermoelasticity, the relation between the various kinematical quantities and the stress tensor $\underline{\tau}$ is

$$\underline{\tau} = \underline{C}\,\underline{e} = \underline{C}\,[\,\underline{\varepsilon} - \underline{\varepsilon}^*\,] = \underline{C}\,[\mathrm{sym}(\mathrm{grad}(\underline{u})) - \underline{\varepsilon}^*\,] \tag{4}$$

In the absence of body forces, the local equations of equilibrium may thus be written in any of the following forms:

$$\mathrm{div}\,\underline{\tau} = 0 \tag{5}$$

$$\mathrm{div}\,(\underline{C}\,\underline{\varepsilon}) = \mathrm{div}(\underline{C}\,\underline{\varepsilon}^*) \tag{6}$$

$$\mathrm{div}\,[\underline{C}\,\mathrm{sym}(\mathrm{grad}(\underline{u}))] = \mathrm{div}(\underline{C}\,\underline{\varepsilon}^*) \tag{7}$$

Here, div(.), grad(.) and sym(.) are the divergence, the gradient and the symmetric part operators.

Appropriate boundary conditions for the field equations are specified as

$$\underline{\tau}\,\underline{n} = \hat{\underline{t}} \qquad \text{on} \qquad \delta B_t \tag{8}$$

where $\underline{n}$ is the outward unit normal, and

$$\underline{u} = \hat{\underline{u}} \qquad \text{on} \qquad \delta B_u \tag{9}$$

Here, $\hat{\underline{t}}$ and $\hat{\underline{u}}$ are assigned tractions and displacement vectors, respectively, and δB_t ,

δB_u are complementary portions of δB.

In general, stress is generated whenever the thermal strain $\underline{\varepsilon}^*$ is non-uniform, in its thermal variation component δT, in the thermal expansion $\underline{\alpha}$, or in both.

Conditions for zero strain

The stress-yielding expression reduces to

$$\underline{\tau} = - \underline{C}\, \underline{\alpha}\, \delta T, \tag{10}$$

only when $\underline{\varepsilon} = 0$, as may be seen from (4) and (1). For this to be the actual solution, it is necessary that the equilibrium requirement

$$\mathrm{div}(\underline{C}\, \underline{\varepsilon}^*) = 0, \tag{11}$$

be satisfied, and the boundary conditions (8) - (9) be met. In particular, the strain vanishes for homogeneous materials with zero displacements prescribed on the entire boundary, and uniform thermal loading. In general, condition (11) is violated, and thus equation (10) is not applicable, if the thermal strain is non-uniform or the material properties vary with position (and/or with temperature), or both. For multi-phase structures, even the satisfaction of (11) and the boundary conditions under the assumption of zero strain does not assure the vanishing of the strains, as continuity conditions must also be satisfied. For instance, in a structure undergoing a uniform temperature variation, continuity of the traction components of the stress (i.e., the condition of equilibrium) is not satisfied at the interface between two phases with different thermal expansions. Thus, for such situations equations (10) - (11) are not applicable.

The isotropic relation

$$\sigma = - E \alpha \delta T, \tag{12}$$

is frequently encountered. To avoid further misuses, it is here emphasized that (12) is applicable only when the eigenstrained body is fully constrained against deformation in the axial direction, and the orthogonal lateral surfaces are stress-free. Under these assumptions, the axial stress (12) will be the only non-vanishing stress component, provided (11) is satisfied. For homogeneous media this condition is verified if and only if the thermal variation is spatially uniform.

THE BI-COATED SPHERE SUBJECT TO PHASE-WISE UNIFORM THERMAL VARIATIONS

Exact solution

A structure composed by a sphere, surrounded by two concentric spherical shells is here considered. The external radii of the spherical core and the two successive shells are r_1 , r_2 and r_3 . The region $r_{i-1} < r < r_i$ (hereafter referred to as 'the i-th substructure') is subject to the uniform temperature variations C_i (Notation: $r_0 = 0$). The constituent material of each substructure is isotropic and homogeneous.

The assumption of material isotropy and the polar symmetry of the problem reduce the equilibrium requirements (7) for the i-th substructure to the single equation

$$\frac{d^2u^i}{dr^2} + \frac{2}{r}\left(\frac{du^i}{dr} - \frac{u^i}{r}\right) = 0 \tag{13}$$

in the i-th phase radial displacement u^i . This equation is expressed in a natural spherical polar coordinate system (r, ϕ, θ), which is employed throughout the present work. Equation (13) is satisfied by taking

$$u^i = K_{i1}\, r + \frac{K_{i2}}{r^2} \tag{14}$$

where the K_{ij} are constants of integration. The non-vanishing stresses corresponding to this displacement are

$$\tau^i_{rr} = -\, 3\, k_i\, \{\alpha_i\, C_i - K_{i1}\} - 4\mu_i \frac{K_{i2}}{r^3} \tag{15}$$

$$\tau^i_{\phi\phi} = \tau^i_{\theta\theta} = -\, 3\, k_i\, \{\alpha_i\, C_i - K_{i1}\} + 2\mu_i \frac{K_{i2}}{r^3} \tag{16}$$

where k_i and μ_i are the bulk and shear moduli of the i-th substructure, respectively. The constants of integration are deduced by imposing continuity, equilibrium, and boundedness conditions:

The vanishing of the radial stress at the free surface implies that

$$K_{31} = \alpha_3\, C_3 + \frac{4\, K_{32}\, \mu_3}{3\, k_3\, r_3^3} \tag{17}$$

The continuity of the radial stress at the interfaces between the layers 1 and 2 and the layers 2 and 3 implies that

$$K_{21} = \alpha_2 C_2 + \left\{ \frac{k_1}{k_2}(K_{11} - \alpha_1 C_1) + \frac{1}{3\,(r_2^3 - r_1^3)\, k_2} \left[4 K_{32} \mu_3 \frac{(r_2^3 - r_3^3)}{r_3^3} - 3\, k_1 (K_{11} - \alpha_1 C_1) r_2^3 \right] \right\} \tag{18}$$

$$K_{22} = \frac{r_1^3}{\mu_2\, (r_2^3 - r_1^3)} \left\{ K_{32}\, \mu_3 \frac{(r_2^3 - r_3^3)}{r_2^3} - \frac{3\, k_1}{4} (K_{11} - \alpha_1\, C_1)\, r_2^3 \right\}; \tag{19}$$

The boundedness of the displacement at $r = 0$ implies that $K_{12} = 0$; introducing the new quantity

$$\bar{K}_{11} = K_{11} - \alpha_1 C_1, \tag{20}$$

the stresses may be rewritten in term of two constants only, as:

$$\tau^1_{rr} = \tau^1_{\phi\phi} = \tau^1_{\theta\theta} = 3\, k_1\, \bar{K}_{11} \tag{21}$$

$$\tau^2_{rr} = 3\, k_1\, \bar{K}_{11} \left(1 - \frac{1 - \frac{r_1^3}{r^3}}{1 - \frac{r_1^3}{r_2^3}} \right) + 4\mu_3\, K_{32} \frac{\left(1 - \frac{r_1^3}{r^3}\right)\left(\frac{r_2^3}{r_1^3} - 1\right)}{(r_2^3 - r_1^3)} \tag{22}$$

$$\tau^2_{\phi\phi} = \tau^2_{\theta\theta} = 3\, k_1\, \bar{K}_{11} \left(1 - \frac{1 + \frac{r_1^3}{2\, r^3}}{1 - \frac{r_1^3}{r_2^3}} \right) + 4\mu_3\, K_{32} \frac{\left(1 + \frac{r_1^3}{2\, r^3}\right)\left(\frac{r_2^3}{r_3^3} - 1\right)}{(r_2^3 - r_1^3)} \tag{23}$$

$$\tau^3_{rr} = 4\mu_3\, K_{32} \left(\frac{1}{r_3^3} - \frac{1}{r^3} \right) \tag{24}$$

$$\tau^3_{\phi\phi} = \tau^3_{\theta\theta} = 4\mu_3\, K_{32} \left(\frac{1}{r_3^3} + \frac{1}{2\, r^3} \right) \tag{25}$$

By imposing continuity of the displacement at the 1-2 and 2-3 interfaces it is then found that

$$\bar{K}_{11} = - \frac{N_1}{D} \tag{26}$$

$$K_{32} = \frac{N_5}{D} \tag{27}$$

where the following definitions were introduced:

$$
\begin{aligned}
D &= f_1\, r_2^6 + f_2\, r_1^3\, r_2^3 + f_3\, r_1^3\, r_3^3 + f_4\, r_2^3\, r_3^3 \\
f_1 &= -\,4\, \bar{\alpha}_{12}\, \mu_3\, \Delta\beta_{32} \\
f_2 &= -\,4\, \bar{\alpha}_{32}\, \mu_3\, \Delta\beta_{21} \\
f_3 &= 4\, \beta_3\, \Delta\mu_{32}\, \Delta\beta_{21} \\
f_4 &= \bar{\alpha}_{12}\, \beta_3 \bar{\alpha}_{23}
\end{aligned}
\tag{28}
$$

$$
N_1 = 4\{\Delta\gamma_{12}\, \beta_2[\Delta r_{21}^3(4\mu_3\, \mu_2\, r_2^3+\mu_2\, \beta_3\, r_3^3)+\mu_3\, \beta_3\, r_1^3\, \Delta r_{32}^3]+\mu_3\, \beta_3\, r_2^3\, \Delta r_{32}^3[\Delta\gamma_{23}\, \beta_2+\Delta\gamma_{13}\, 4\mu_2]\}
\tag{29}
$$

$$
N_5 = \beta_3 r_2^3 r_3^3\, \{2\Delta\gamma_{23}\, \mu_2(\beta_1+2\beta_2)\Delta r_{21}^3+3\beta_1\, [(\Delta\gamma_{23}\, r_2^3 +\Delta\gamma_{12}\, r_1^3)\lambda_2+\Delta\gamma_{13}\, 2\mu_2\, r_1^3]\}
\tag{30}
$$

$$
\begin{aligned}
&\beta_i = 2\, \mu_i + 3\, \lambda_i = 3\, k_i \\
&\bar{\alpha}_{ij} = \beta_i + 4\, \mu_j \\
&\gamma_i = \alpha_i\, C_i \\
&\Delta x_{ij} = x_i - x_j\,, \qquad\qquad x = \gamma,\, \mu,\, \beta,\, r^3
\end{aligned}
\tag{31}
$$

Substitution of (26) - (31) into (21) - (25) and (14) yields all stresses and displacements, respectively.

The thin film case

For the purpose of thin film analysis, the coating radii are expressed as

$$
r_2 = r_1\, (1+x),\ r_3 = r_1\, (1 + px), \qquad 1 \leqq p \leqq 10
\tag{32}
$$

In the limit as x approaches zero, it is then found that

$$\bar{K}_{11} = f_{11}\, x \tag{33}$$

$$K_{32} = f_{50} + f_{51}\, x \tag{34}$$

where higher order terms were neglected, and the definitions

$$f_{11} = -4\frac{\Delta\gamma_{13}[(p-1)z_2\beta_3\mu_3+\Delta\gamma_{12}z_3\beta_2\mu_2]}{\beta_1 z_2 z_3} \tag{35}$$

$$f_{50} = \frac{\beta_3}{3\, z_3}\Delta\gamma_{13}r_1^3 \tag{36}$$

$$f_{51} = \beta_3\frac{\Delta\gamma_{13}[(p-1)z_2\beta_3(\beta_1+4\mu_3)+\beta_1 z_3(3\beta_2+8\mu_2)]+\Delta\gamma_{23}\beta_2\beta_1 z_3+4\Delta\gamma_{12}z_3\beta_2\mu_2}{3\beta_1 z_2 z_3^2}\, r_1^3 \tag{37}$$

$$z_i = 2\,\mu_i + \lambda_i \tag{38}$$

were introduced.

APPLICATION: A CERAMIC-COATED METAL STRUCTURE WITH OXIDATION BARRIER AS INTERMEDIATE LAYER

The case of a Nickel superalloy sphere with a plasma-sprayed Zirconia coating and a MCrAlY bonding layer is studied next. Table 1 reports the defaults values for the geometric, material, and processing parameters employed [Lombard (1985), Schmauder and Schubert (1986), Schubert (1986)]. The dependence of the transverse and radial stresses on several of these parameters is studied by varying one of them at the time, as summarized in Table 2.

The first parameters considered are the Poisson's ratios of the oxidation barrier and of the coating, as the lamellar microstructure induced by some processing conditions makes the latter fluctuate considerably [Lombard (1985)]. Figure 1 shows that varying the Poisson's ratio of the intermediate layer reduces the transverse stress there, but bears no significant effect on the transverse stress state of the coating. The viceversa is also true. This substantial decoupling is a consequence of the relative thinness of the coatings, as discussed in the last section. Another consequence of the thin geometry is that the radial stresses are negligible, compared with the transverse ones, as exhibited in Figure 1.b. In view of this, radial stresses are not discussed any further.

Figure 2 displays the stresses at the mid-point of each of the three phases as a function of the substrate temperature during deposition. The importance of this control parameter is obvious: Allowing the substrate to heat during deposition induces moderate compressive stresses, while low substrate temperatures correspond to high tensile stresses in both the intermediate layer and the coating.

Table 2 compares the stresses in the default system (Case 1) with the stresses obtained by varying the intermediate layer's thickness, temperature variation, or thermal expansion. The imposed variations alter the stress level of the oxidation barrier significantly (especially in Case 2, where $\Delta\gamma_{12}$ is nearly zero, and in Case 3, where it becomes large and negative), but have a minor effect on the coating stress.

DISCUSSION AND CONCLUSIONS

The exact thermoelastic solution for sphere with three concentric phases, subject to a phase-wise homogeneous temperature variation was presented in this paper. Concerning this solution, it is observed that all stresses vanish if and only if $\gamma_1 = \gamma_2 = \gamma_3$. Also, it is seen by (24) - (25), that the radial and transverse stresses in the outermost layer are always of opposite sign. This is not true for the intermediate layer, as shown by a later counterexample, and is trivially true for the substrate, since these stresses here coincide.

Algebraic manipulation proves D, -see eq. (28) - to be positive definite. Thus, the substrate stresses are compressive if and only if N_1 is positive, which is in turn true if $\gamma_3 < \gamma_2 < \gamma_1$. Similarly, the outermost layer is in transverse compression (and radial tension) if $\gamma_3 > \gamma_2 > \gamma_1$.

For the special case $C_2 = C_3 = 0$, the solution of Luo and Weng (1987) is recovered. For $r_1 = r_2 = r_3$ the solution of Boley and Weiner (1985) is obtained.

The exact solution was employed to determine the stress level in a Nickel superalloy structure, with a bi-layered plasma-sprayed coating, consisting of an internal oxidation barrier and a Zirconia thermal barrier coating. For the system studied, the thermoelastic moduli of the oxidation barrier, its thickness, and its thermal load are found not to affect the coating stresses significantly, in accordance with experimental reports [Hobbs and Reiter (1988)].

The dominant control parameters, for the minimisation of the coating stresses in the system examined, are the substrate temperature - substrate cooling inducing compression - and the coating's Poisson' ratio. The thin film limit of the discussed exact solution was deduced in a preceding section . In this context, it is observed that:

(i) the radial stresses in the coatings are negligible magnitude-wise, with respect to the transverse ones.

(ii) the thermoelastic properties of the intermediate layer, and its thermal load, affect the stresses in the outermost layers only in first order in x, and thus are irrelevant in the thin film limit.

(iii) the sign of K_{32}, and thus the compressive or tensile nature of the coating stresses is dominated by $\Delta\gamma_{13}$, and not by $\alpha_1 - \alpha_3$, as incorrectly reported in Takeuchi et al. (1990).

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SUMMARY

The thermoelastic problem of a three-phase concentric sphere subject to phase-wise uniform temperature variations is solved exactly. With this solution, the cooldown stresses in a metallic structure with plasma-sprayed oxidation- and thermal-barrier coatings are determined. The general thin-film approximation to the subject problem is presented.

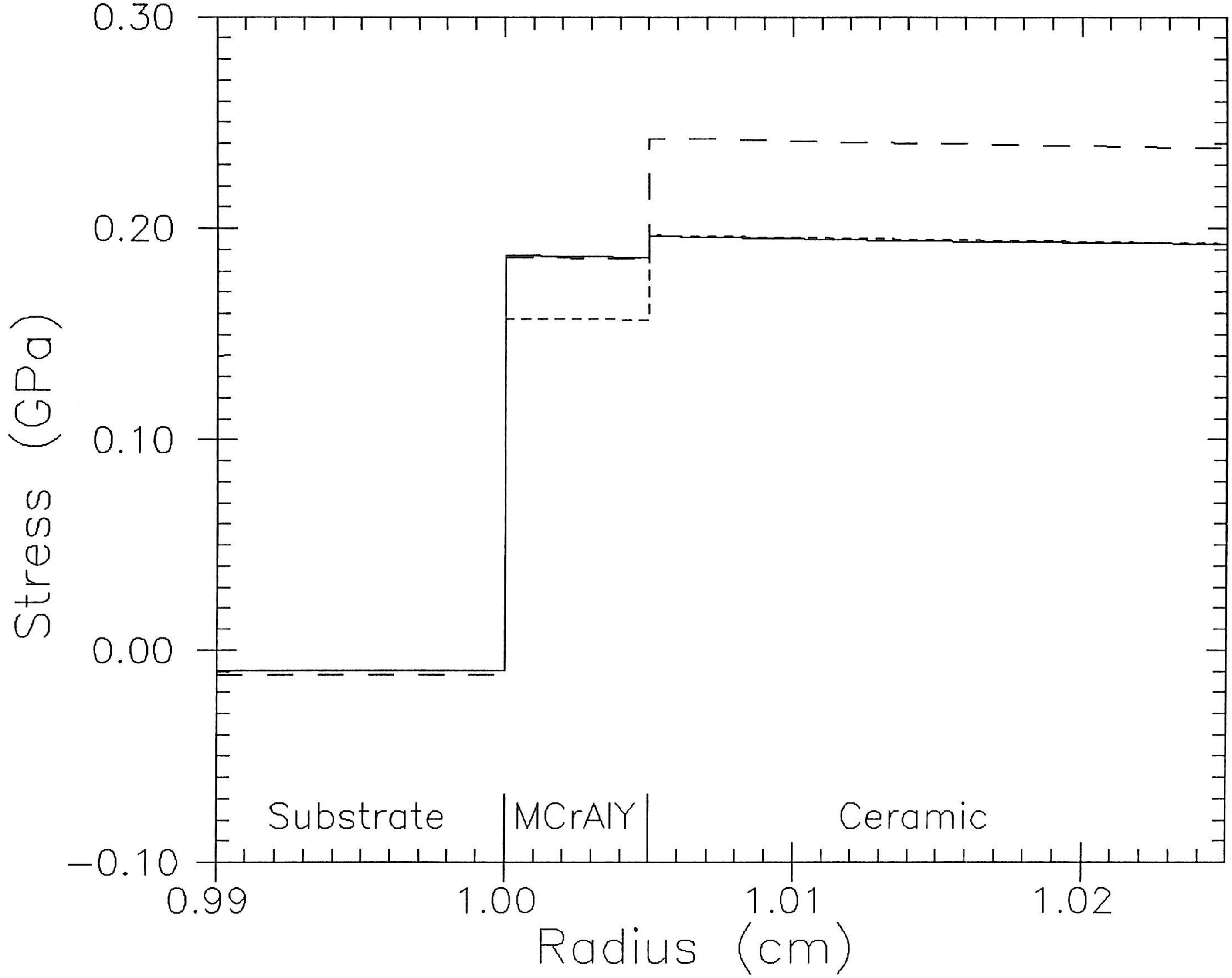
Key words: Thermal Stress, Coating, Layered Structure.

FIGURE CAPTIONS AND TABLES

Figure 1. Effect of the Poisson's ratios on the transverse (a) and radial (b) thermal stress in the coated sphere; (—— Case 1, see Table 1; – – – Case 2, as Case 1, but ν_3 = .26; ------ Case 3, as Case 1, but ν_2 = .1).

Figure 2. Transverse thermal stress vs. substrate temperature during deposition (Case 1 system - see Table 1).

Figure 1 (a).



0.30
0.20
0.10
0.00
−0.10
Stress (GPa)
Substrate
MCrAlY
Ceramic
0.99
1.00
1.01
1.02
Radius (cm)

Figure 1 (b).

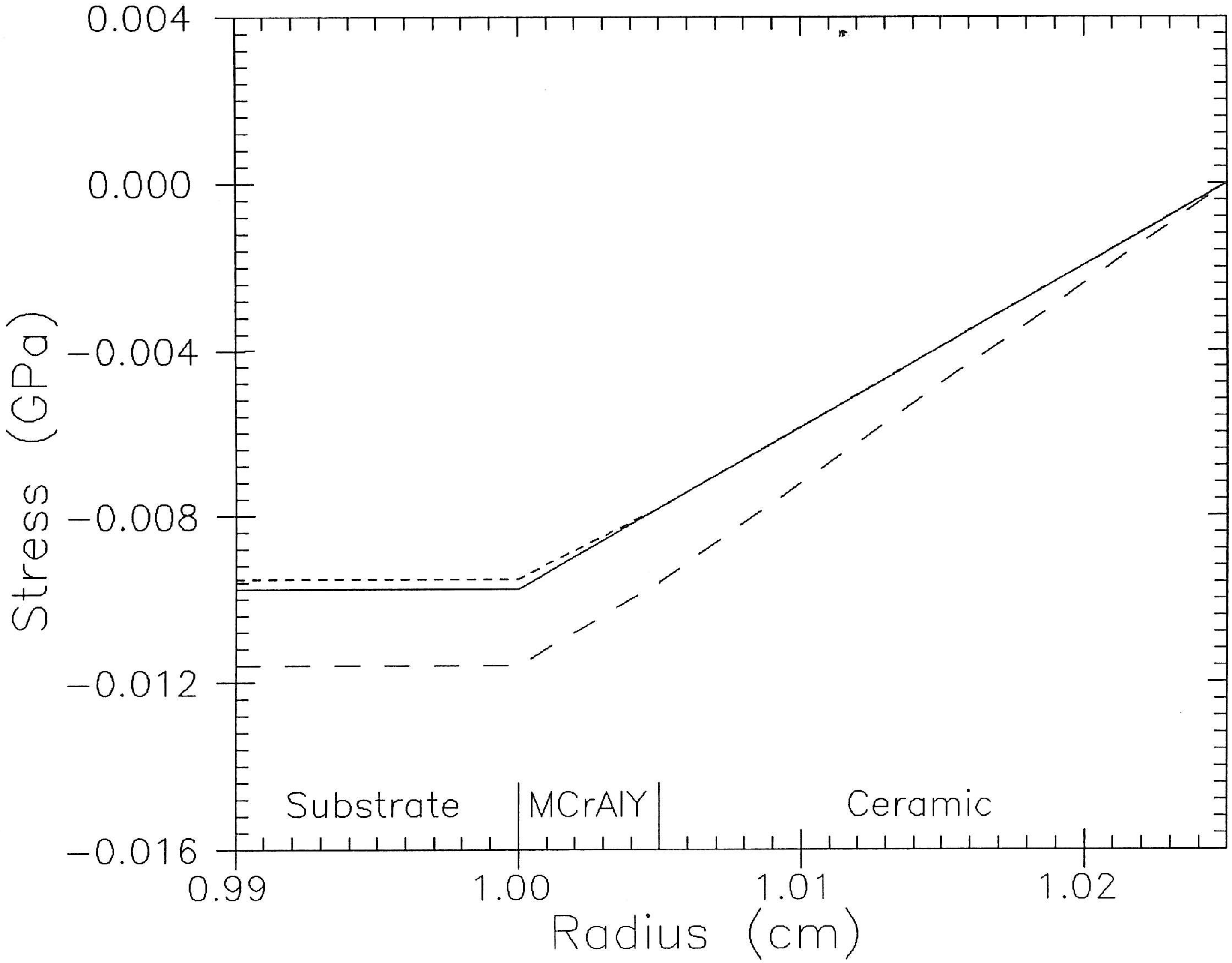
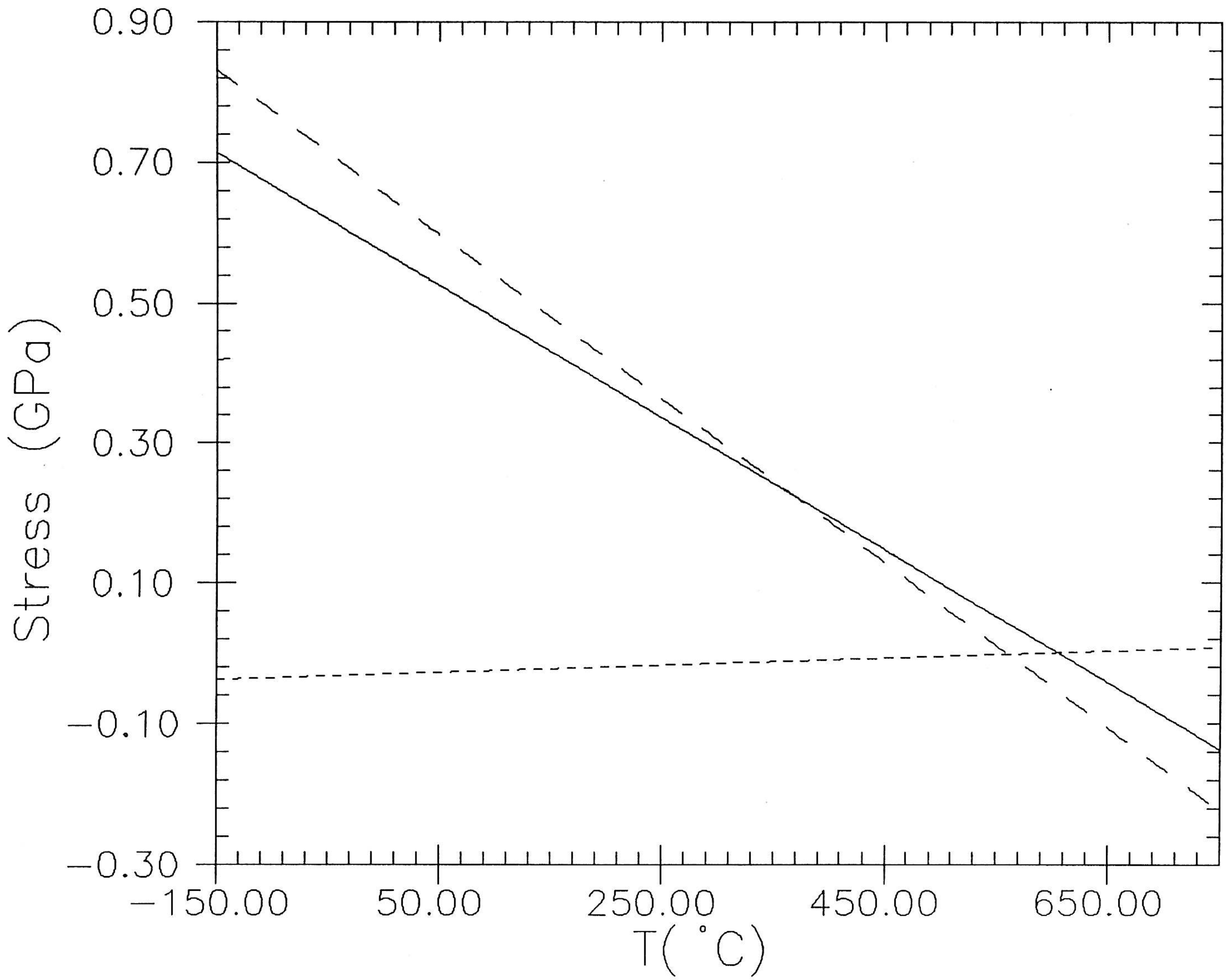

Stress (GPa)
0.004
0.000
−0.004
−0.008
−0.012
−0.016
Substrate
MCrAlY
Ceramic
0.99
1.00
1.01
1.02
Radius (cm)

Figure 2.



Stress (GPa)
0.90
0.70
0.50
0.30
0.10
−0.10
−0.30
−150.00
50.00
250.00
450.00
650.00
T(˚C)

Table 1. Case 1: Material characteristic and processing condition.

Phase (i)	E_i (GPa)	ν_i	α_i (mK^{-1})	C_i (K)	r_i (cm)
1	200	.25	$20\cdot10^{-6}$	-400	1
2	45	.25	$16\cdot10^{-6}$	-700	1.005
3	45	.075	$11\cdot10^{-6}$	-1100	1.025

Table 2. Influence of material characteristic and processing conditions of the bonding layer on the transverse thermal stresses (mid-point values reported).

Case	Stress in the substrate	Stress in the bonding layer	Stress in the ceramic layer
1*	-0.0098 GPa	0.1868 GPa	0.1944 GPa
2#	-0.0079 GPa	-0.0038 GPa	0.1958 GPa
3~	-0.0061 GPa	-0.1880 GPa	0.1973 GPa
4&	-0.0152 GPa	0.1827 GPa	0.1900 GPa

*See Table 1.

#As Case 1, but C_2 = - 500 K.

~As Case 1, but $\alpha_2 = 7\cdot10^{-6}$ mK^{-1}.

&As Case 1, but r_2 = 1.02 cm, r_3 = 1.04 cm.

APPENDIX II. NOTATION

The following symbols are used in this paper:

B = region occupied by material subject to thermal strain field;

$\underline{C}$ = stiffness tensor;

C_i = uniform temperature variation in the i-th substructure;

D = constant, see (28);

div(.) = divergence operator;

$\underline{e}$ = mechanical component of strain tensor;

E = Young's modulus;

f_i = constant, see (28);

f_{ij} = constant, see (35)-(37);

grad(.) = gradient operator;

k_i = bulk modulus of i-th substructure;

K_{ij} = integration constant, see (14);

$\breve{K}_{11}$ = constant, see (20);

$\underline{n}$ = outward unit normal on δB;

N_i = constant, see (29) - (30);

p = thickness parameter, see (32);

r, θ, ϕ = polar coordinates;

r_i = external radius of the i-th substructure;

sym(.) = symmetric part operator;

$\hat{\underline{t}}$ = assigned traction vector;

u^i = displacement of the i-th substructure;

$u_{i,j}$ = partial derivative of u_i respect to x_j;

x = thickness parameter, see (32);

z_i = material constant, see (38);

α = isotropic thermal expansion coefficient;

$\underline{\alpha}$ = thermal expansion tensor;

α_i = thermal expansion coefficient of the i-th substructure;

$\bar{\alpha}_{ij}$ = material constant, see (31);

β_i = material constant, see (31);

δB = boundary of region B;

δB_t, δB_u = complementary portions of δB;

δT = temperature variation field;

$\Delta\beta_{ij}$, $\Delta\gamma_{ij}$, $\Delta\mu_{ij}$, Δr^3_{ij} = see (31) for definitions;

$\underline{\varepsilon}$ = strain tensor;

$\underline{\varepsilon}^*$ = thermal component of strain tensor;

γ_i = constant, see (31);

λ_i, μ_i = Lamé constants of the i-th substructure;

ν_i = Poisson's ratio;

σ = stress;

$\underline{\tau}$ = stress tensor;

τ^i_{rr}, $\tau^i_{\phi\phi}$, $\tau^i_{\theta\theta}$ = normal stresses in the i-th substructures along r, ϕ, θ, directions;