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APPROXIMATE EVALUATION OF THE ELASTIC INTERFACIAL STRESSES IN THIN FILMS WITH APPLICATION TO HIGH-T_c SUPERCONDUCTING CERAMICS

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Abstract—The mechanical strength and structural integrity of a high-T_c superconductor may play a decisive role when a superconducting material is used for practical purposes. In this analysis, we suggest a simple analytical model for an approximate evaluation of the elastic thermal stresses in elongated thin films in application to high-T_c superconducting ceramics. The emphasis is on interfacial shearing and peeling stresses responsible for the integrity of the film–substrate composite and the strength of the intermediate material, if any. A numerical example is performed for a superconducting ceramic $YBa_2Cu_3O_{7-\delta}$ deposited on a Si, GaAs, Al_2O_3 or MgO substrate. It is shown that the thermally-induced stresses and strains can be brought down by reducing the thermal expansion (contraction) mismatch of the film and the substrate, the fabrication temperature, and Young's modulus of the film material. Our theory is equally applicable to other film structures as long as the materials involved can be treated as linearly elastic.

INTRODUCTION

In potential applications, the recently discovered high transition temperature (high-T_c) ceramic superconductors (Bednorz and Müller, 1986; Wu *et al.*, 1987; Cava *et al.*, 1987) may experience large mechanical stresses and strains. These could be imposed by magnet fabrication, high magnetic fields, and, in the case of superconducting films, also by thermal contraction mismatch with the substrate material (see, for instance, Baynham, 1988; Severin and de With, 1988). Although the mechanical strength of a superconductor may appear to be not as important a property as, say, the high superconducting transition temperature, high upper critical magnetic field or high critical current density, it may play a decisive role when a superconducting material is used for practical purposes. Since ceramics are brittle materials, and break quite easily when stretched, bent or hit, the use of ceramics as practical superconductors requires that they possess high ultimate stress and strain, sufficient fracture toughness, and good shock resistance. It is also important that the actual stresses and strains at low temperatures can be predicted and, if possible, minimized.

In the analysis below we suggest a simplified analytical model for an approximate evaluation of the elastic thermally-induced stresses in superconducting ceramic films fabricated on thick substrates. As is known, thin films exhibit the best superconducting properties and are useful not only for potential applications in electronic devices, but also for the access they lend to certain experiments which otherwise would be difficult to perform (see, for instance, Park *et al.*, 1988).

The approach taken in this paper enables one to satisfy the boundary conditions at the film edges within the framework of an elementary beam (long-and-narrow plate) theory and therefore is thought to provide a reasonable compromise between the simplest strength-of-materials stress models where these conditions are not considered, and rigorous but complicated solutions based on methods of mathematical physics.

Note that mechanical properties of high-temperature superconductors, as well as various mechanical aspects of fabrication and physical properties of superconducting films, were investigated by many authors (see References). The mechanical behavior of superconducting ceramic films was studied first by Lau and Moresco (1988) on the basis of the finite element method. The present analysis seems to be the first attempt to apply analytical methods of engineering mechanics to the problem in question.

It should be pointed out that although our theory is developed for superconducting films, it is equally applicable to films made of other nonorganic or organic materials, as long as the linear elastic approach can be used.

THEORY

We proceed from the following coupled differential equations for the interfacial stresses in elongated bi-material plates experiencing temperature change (Suhir, 1989):

$$\left.\begin{aligned} \tau''(x)-k^2\tau(x) &= \frac{\mu}{K\kappa}p'''(x) \\ p^{\mathrm{IV}}(x)+4\alpha^4 p(x) &= 4\mu\alpha^4\tau'(x) \end{aligned}\right\}. \tag{1}$$

In these equations, $\tau(x)$ is the shearing stress, $p(x)$ is the "peeling" (normal) stress,

$$K=\left(\frac{1-\nu_1^2}{E_1}h_1+\frac{1-\nu_2^2}{E_2}h_2\right)^{-1} \tag{2}$$

is the spring constant (through-thickness stiffness) of the composite,

$$\kappa=\frac{h_1}{3G_1}+\frac{h_2}{3G_2} \tag{3}$$

is the interfacial compliance (Suhir, 1986), E_1 and E_2 are Young's moduli of the materials, ν_1 and ν_2 are their Poisson's ratios,

$$G_1=\frac{E_1}{2(1+\nu_1)} \quad \text{and} \quad G_2=\frac{E_2}{2(1+\nu_2)}$$

are the shear moduli, h_1 and h_2 are the thicknesses of the composite plates,

$$\mu=\frac{h_1D_2-h_2D_1}{2D} \tag{4}$$

is a parameter of the relative flexural rigidity of the plates,

$$D_1=\frac{E_1h_1^3}{12(1-\nu_1^2)} \quad \text{and} \quad D_2=\frac{E_2h_2^3}{12(1-\nu_2^2)}$$

are their cylindrical rigidities, $D=D_1+D_2$ is the total cylindrical rigidity,

$$k=\sqrt{\frac{\lambda}{\kappa}} \tag{5}$$

is the parameter of the longitudinal compliance,

$$\alpha=\sqrt[4]{\frac{KD}{4D_1D_2}} \tag{6}$$

is the parameter of the through-thickness compliance, and

$$\lambda = \frac{1-\nu_1^2}{E_1 h_1} + \frac{1-\nu_2^2}{E_2 h_2} \tag{7}$$

is the longitudinal axial compliance of the plate.

In the case of a thin film of thickness h_1 and a substrate of a significantly larger thickness h_2 (Fig. 1), formulae (2), (3) and (4) yield:

$$K = \frac{E_2}{(1-\nu_2^2)h_2}, \quad \kappa = \frac{2(1+\nu_2)}{3E_2}h_2, \quad \mu = \frac{h_1}{2}, \tag{8}$$

so that the coefficient in the right part of the first equation in (1) becomes proportional to the film thickness:

$$\frac{\mu}{K\kappa} = \sim h_1. \tag{9}$$

Since this thickness is small, in a simplified analysis one can use the homogeneous equation

$$\tau''(x) - k^2\tau(x) = 0 \tag{10}$$

to evaluate the shearing stress. This equation reflects an obvious assumption that the peeling stress has an insignificant effect on the shearing stress.

Equation (10) has the following solution

$$\tau(x) = C_1 \sinh kx, \tag{11}$$

where the other constant of integration is put equal to zero to make the distribution of the shearing stress antisymmetric with respect to the origin $x = 0$. The constant C_1 can be determined from the boundary condition (Suhir, 1986):

$$\tau'(l) = \frac{\Delta\alpha\Delta t}{k\kappa \cosh kl} = k\frac{\Delta\alpha\Delta t}{\lambda \cosh kl}, \tag{12}$$

so that the shearing stress is distributed along the film–substrate interface in accordance with the equation

$$\tau(x) = \tau_{\max}\chi_\tau(x), \tag{13}$$

where

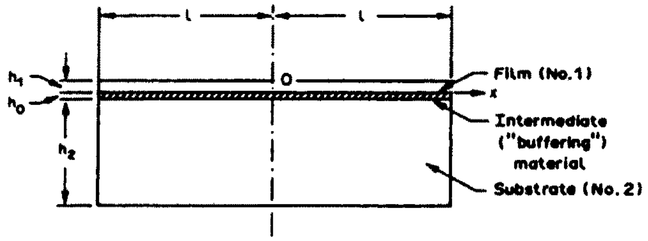


Fig. 1. Film–substrate composite.

$$\tau_{max} = k\frac{\Delta\alpha\Delta t}{\lambda}\tanh kl \tag{14}$$

is the maximum value of the shearing stress at the end cross-section, and the function

$$\chi_\tau(x) = \frac{\sinh kx}{\sinh kl} \tag{15}$$

reflects the longitudinal distribution of this stress.

Note that eqn (10) can be obtained from the first equation in (1) assuming that the spring constant K in the through-thickness direction is infinitely large: $K \to \infty$. In this case the parameter α is also infinitely large, and the second equation in (1) yields:

$$p_\infty(x) = p(x)|_{K\to\infty} = \mu\tau'(x) = p^\infty_{max}\chi^\infty_p(x), \tag{16}$$

where

$$p^\infty_{max} = \mu\frac{\Delta\alpha\Delta t}{\kappa} \tag{17}$$

is the maximum peeling stress in the case of an infinitely large through-thickness stiffness, and the function

$$\chi^\infty_p(x) = \frac{\cosh kx}{\cosh kl} \tag{18}$$

reflects the distribution of this stress along the interface.

Using (16), we rewrite the second equation in (1) as follows:

$$p^{IV}(x) + 4\alpha^4 p(x) = 4\alpha^4 p_\infty(x). \tag{19}$$

The solution to this equation can be presented in the form

$$p(x) = \frac{s^4}{1+s^4}p^\infty_{max}[\chi^\infty_p(x) + A_0V_0(\alpha x) + A_2V_2(\alpha x)], \tag{20}$$

where the parameter

$$s = \frac{\alpha\sqrt{2}}{k} \tag{21}$$

reflects the effect of the ratio of the through-thickness and the longitudinal stiffnesses. The functions $V_0(\alpha x)$ and $V_2(\alpha x)$ are expressed as

$$V_0(\alpha x) = \cosh\alpha x\cos\alpha x, \quad V_2(\alpha x) = \sinh\alpha x\sin\alpha x,$$

and obey the following convenient rules of differentiation:

$$V_0'(\alpha x) = -\alpha\sqrt{2}V_3(\alpha x), \quad V_1'(\alpha x) = \alpha\sqrt{2}V_0(\alpha x),$$
$$V_2'(\alpha x) = \alpha\sqrt{2}V_1(\alpha x), \quad V_3'(\alpha x) = \alpha\sqrt{2}V_2(\alpha x),$$

where

$$V_{1,3}(\alpha x) = \frac{1}{\sqrt{2}}(\cosh \alpha x \sin \alpha x \pm \sinh \alpha x \cos \alpha x).$$

Equation (19) can be presented, by integrations, as follows:

$$p''(x) = 4\alpha^4\left[-\int_{-l}^{x}\int_{-l}^{\xi} p(\xi')\,\mathrm{d}\xi'\,\mathrm{d}\xi + T(x)\right],$$

where

$$T(x) = \int_{-l}^{x} \tau(\xi)\,\mathrm{d}\xi \tag{22}$$

is the longitudinal force in the film. Both terms in the brackets in the above equation turn to zero at the end cross-section $x = l$, and, therefore,

$$p''(l) = 0.$$

This boundary condition, together with the condition

$$\int_{-l}^{l} p(x)\,\mathrm{d}x = 0$$

of self-equilibrium, results in the following values of the constants A_0 and A_2 of integration:

$$A_0 = 2\sqrt{2}\,\frac{V_3(v) - s^3 V_0(v)\tanh u}{s^2(\sinh 2v + \sin 2v)}, \quad A_2 = -2\sqrt{2}\,\frac{V_1(v) + s^3 V_2(v)\tanh u}{s^2(\sinh 2v + \sin 2v)}, \tag{23}$$

where $u = kl$, $v = \alpha l$.

For sufficiently large u and v values, i.e. for relatively stiff and long composite structures, formulae (23) can be simplified:

$$A_0 \cong \frac{2}{s^2}\mathrm{e}^{-v}[\sin v - (s^3 + 1)\cos v], \quad A_2 \cong \frac{2}{s^2}\mathrm{e}^{-v}[\cos v + (s^3 + 1)\sin v].$$

In this case the peeling stress $p(x)$ can be presented as follows:

$$p(x) = p_{\infty}(x)\phi(\alpha, x), \tag{24}$$

where the function

$$\phi(\alpha, x) = \frac{s^4}{1+s^4}\left[1 - \mathrm{e}^{-(\alpha-k)(l-x)}\,\frac{(s^3+1)\cos\alpha(l-x) - \sin\alpha(l-x)}{s^2}\right] \tag{25}$$

accounts for the effect of the finite through-thickness stiffness. Obviously, this function trends to unity when the spring constant K trends to infinity. In thin-film structures, the parameter α of the through-thickness stiffness is significantly greater than the parameter k of the longitudinal interfacial stiffness, and therefore the ratio s is substantially larger than unity. Then formula (25) can be simplified as follows:

$$\phi(\alpha, x) = 1 - e^{-\alpha(l-x)}\left[s\cos\alpha(l-x) - \frac{\sin\alpha(l-x)}{s^2}\right]. \tag{26}$$

The function $\varphi(\alpha, x)$ is plotted in Fig. 2. As evident from this figure, for small enough x values, i.e. for cross-sections sufficiently remote from the film ends, the function ϕ is close to unity, and therefore the peeling stress can be quite accurately predicted by formula (16) assuming infinitely large through-thickness stiffness. On the other hand, for cross-sections close to the film ends, the factor $\phi(\alpha, x)$ can be presented as

$$\phi \cong 1 - s[1 - \alpha(l-x)]. \tag{27}$$

At the end $x = l$ this factor becomes equal to

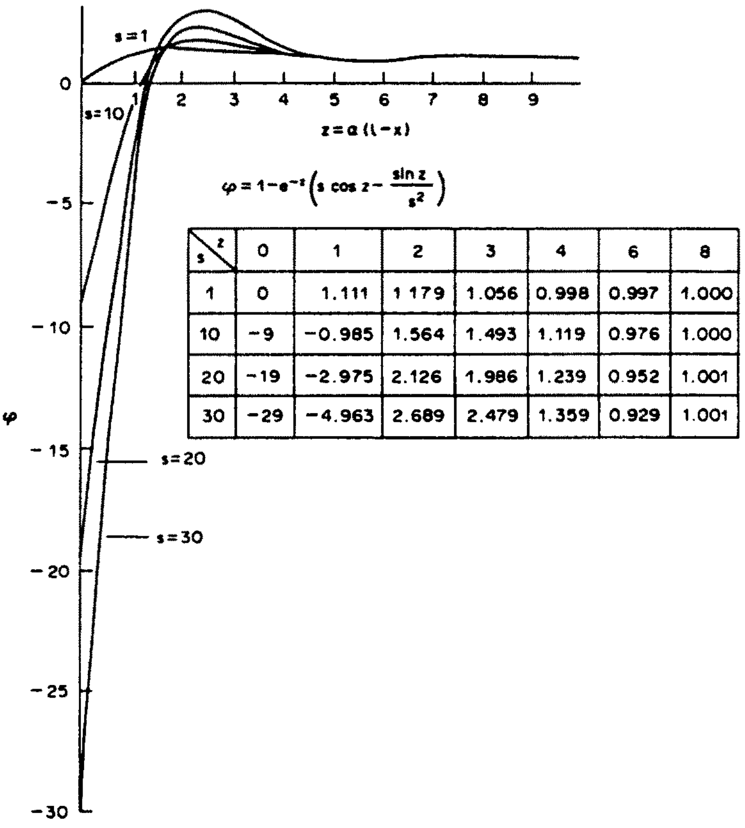
$$\phi = 1 - s, \tag{28}$$

so that its absolute value can be substantially greater than unity. Note that formulae (27) and (28) can be used only for moderately large α values, since, as was shown above, the function ϕ trends to unity if the α value trends to infinity.

Assuming that the film is so thin that it does not experience bending stress at all, one can evaluate the tensile ("membrane") stress by the formula

$$\sigma_1(x) = \frac{T(x)}{h_1}, \tag{29}$$

where the force $T(x)$ is expressed by (22).



$$\varphi = 1 - e^{-z}\left(s\cos z - \frac{\sin z}{s^2}\right)$$

s \ z	0	1	2	3	4	6	8
1	0	1.111	1.179	1.056	0.998	0.997	1.000
10	−9	−0.985	1.564	1.493	1.119	0.976	1.000
20	−19	−2.975	2.126	1.986	1.239	0.952	1.001
30	−29	−4.963	2.689	2.479	1.359	0.929	1.001

Fig. 2. Peeling stress distribution function.

Table 1. Calculated maximum low temperature stresses for a 1 μm thick superconducting $YBa_2Cu_3O_{7-\delta}$ ceramic film

		Mechanical properties				Calculated parameters					Max. stress (MPa)		
Materials		E (GPa)	ν	$\bar{\alpha}$ (°C^{-1})	Thickness (μm)	$K \times 10^{-14}$ (N m^{-3})	$\kappa \times 10^{14}$ (m^3 N^{-1})	$\alpha \times 10^{-4}$ (m^{-1})	$k \times 10^{-4}$ (m^{-1})	s	σ_{max}	τ_{max}	p_{max}
Substrate (No. 2)	Si	131	0.28	2.9×10^{-6}	508	2.798	0.3309	30.090	4.859	8.758	937.6	45.56	−8.587
	GaAs	86	0.31	5.8×10^{-6}		1.873	0.5159	27.217	3.891	9.892	632.1	24.59	−4.254
	Al_2O_3	255	0.30	6.2×10^{-6}		5.516	0.1726	35.654	6.728	7.494	589.9	39.69	−8.670
	MgO	317	0.29	11.0×10^{-6}		6.813	0.1378	37.587	7.529	7.060	84.3	6.35	−1.448
$YB\alpha_2Cu_3O_{7-\delta}$ (No. 1)		96	0.25	11.8×10^{-6}	1.6								

$$D_1 = \frac{E_1 h_1^3}{12(1-\nu_1^2)}, \quad D_2 = \frac{E_2 h_2^3}{12(1-\nu_2^2)}, \quad K = \frac{12 D_2}{h_2^4},$$

$$\alpha = \frac{1}{h_2}\sqrt[4]{3\frac{D_2}{D_1}}, \quad K \cong \begin{cases} 2(1+\nu_2)h_2/3E_2, & l \gg h_2, \\ (1+\nu_2)(3-\nu_2)l/E_2, & l \ll h_2, \end{cases} \quad \lambda_1 = \frac{1-\nu_1}{E_1 h_1}, \quad k = \sqrt{\frac{\lambda_1}{\kappa}}, \quad s = \frac{\alpha\sqrt{2}}{k},$$

$$\sigma_{max} = \frac{E_1}{1-\nu_1}(\alpha_1 - \alpha_2)\Delta t, \quad \tau_{max} = k h_1 \sigma_{max}, \quad p_{max} = \frac{1-s}{2}(k h_1)^2 \sigma_{max}$$

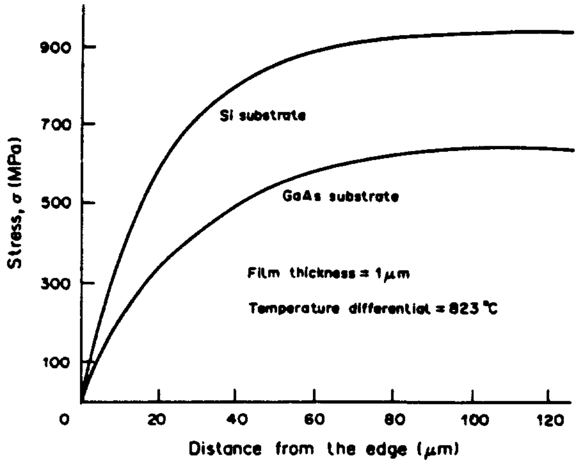


Fig. 3. Stress in a superconducting ceramic film due to its thermal contraction mismatch with the substrate.

NUMERICAL DATA

The numerical examples were carried out for a superconducting ceramic $YBa_2Cu_3O_{7-\delta}$ deposited on different substrates. The input data were taken from the paper by Lau and Moresco (1988). We assumed that the stresses at the deposition temperature 600°C are zero, that no higher temperature anneal is needed, and that the operating temperature of the composite structure is about −223°C, so that the change in temperature causing low temperature stresses is $\Delta t = 823$°C. The material characteristics at −223°C are given in Table 1. Although the mechanical properties of both the film and substrate materials may be time dependent, and, in addition, may exhibit nonlinear behavior, in this analysis we assumed that the material properties are constant in time and that the materials perform elastically. The calculated maximum stress in the film occurs in the case of a silicon substrate and is $\sigma_{max} = 937.6$ MPa. This result is in good agreement with the finite element data which predicted $\sigma_{max} = 931$ MPa (Lau and Moresco, 1988). The distribution of stresses along the film is shown in Fig. 3 for the cases of Si and GaAs substrates.

The interfacial shearing stresses are plotted Fig. 4. These are about 4–8% of the normal

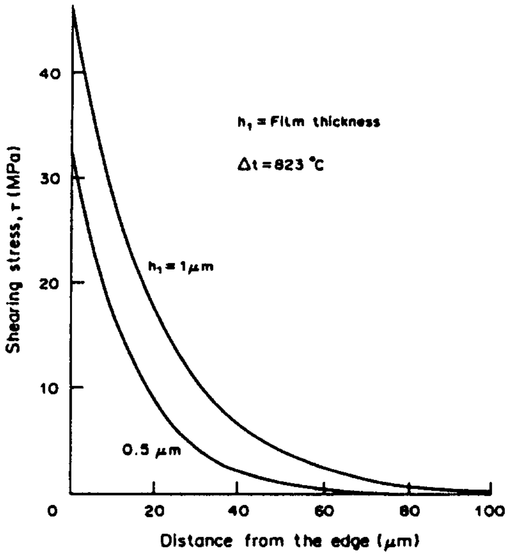


Fig. 4. Interfacial shearing stress.

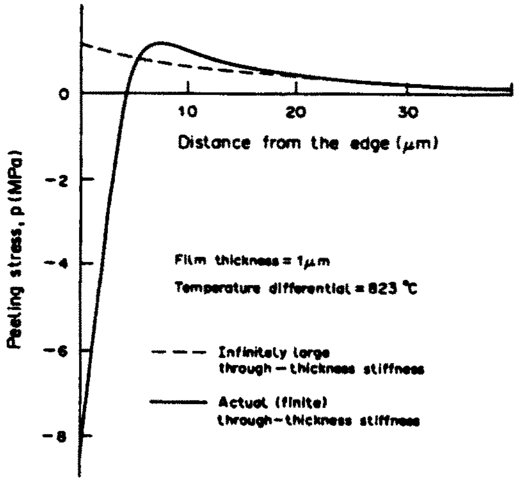


Fig. 5. Interfacial peeling stress.

stresses in the film. The distribution of the peeling stress along the film at the end zones is shown in Fig. 5 for a 1 μm thick film on a Si substrate. These stresses are small and do not exceed 1–2% of the stresses in the film.

In order to determine whether employment of an intermediate material could bring down the stresses, let us examine the buffering effect of a 0.1 μm thick silver layer ($E = 70.4$ MPa, $\nu = 0.35$). Such a layer results in an additional longitudinal compliance at the interface $\kappa_a = 2.557 \times 10^{-18}$ m^3 N^{-1}, and in an additional through-thickness compliance $1/K_a = 1.246 \times 10^{-18}$ m^3 N^{-1}. These values are too small to have an appreciable effect on stresses in long enough films. To assess the film length, a further decrease of which would bring the stresses in the film down, we use formula (14). As follows from this formula, such an effect will take place for kl values smaller than, say, 3. The corresponding calculated film lengths for the Si, GaAs, Al_2O_3 and MgO substrates are 122, 389, 89 and 80 μm, respectively. Therefore, application of intermediate materials as strain buffers is sensible only for very short films.

CONCLUSIONS

The following major conclusions can be drawn from the analysis performed.

- An approximate theory of thermally-induced stresses in thin high-T_c superconducting ceramic films was developed.
- Application of an intermediate buffering material, as far as the stress level in the film is concerned, is advisable only for sufficiently short films, which are characterized by kl values smaller than, say, 3.
- The stresses and strains in the film can be brought down by reducing the thermal expansion (contraction) mismatch of the film and the substrate, the film fabrication temperature and Young's modulus of the film material. It is advisable, if possible, to use substrates whose low temperature coefficients of thermal expansion are somewhat larger than the coefficient of thermal expansion of the film. This will result in compressive stresses in the film, which is a favorable factor, as far as initiation and propagation of brittle cracks are concerned.
- Future work should focus on the consideration of nonlinear and time-dependent effects, as well as on the application of theoretical and experimental methods of fracture mechanics for improved reliability and better understanding of the mechanical behavior of brittle high-T_c superconducting film materials.

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