

A Model for Designing Functionally Gradient Material Joints

An analytical model allows estimation of thermally induced stresses in discrete-layer FGM joints, facilitating design for processing

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ABSTRACT. An analytical, thin-plate layer model was developed to assist research and development engineers in the design of functionally gradient material (FGM) joints consisting of discrete steps between end elements of dissimilar materials. Such joints have long been produced by diffusion bonding using intermediates or multiple interlayers; welding, brazing or soldering using multiple transition pieces; and glass-to-glass or glass-to-metal bonding using multiple layers to produce matched seals. More recently, FGM joints produced by self-propagating high-temperature synthesis (SHS) are attracting the attention of researchers. The model calculates temperature distributions and associated thermally induced stresses, assuming elastic behavior, for any number of layers of any thickness or composition, accounting for critically important thermophysical properties in each layer as functions of temperature. It is useful for assuring that cured-in fabrication stresses from thermal expansion mismatches will not prevent quality joint production. The model's utility is demonstrated with general design cases.

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Introduction

Joining of dissimilar materials into hybrid structures to meet severe design requirements is becoming more necessary and common (Ref. 1). Joints between heat-resistant or refractory metals and refractory or corrosion-resistant ceramics and intermetallics are especially in demand for advanced aerospace engines and airframes, advanced energy generation and conversion system components, chemical processing plant components, and advanced automobile engines (Refs. 2, 3). The drivers for such hybrid structures are multifold and include: 1) optimization of mechanical properties (e.g., strength, modulus, toughness); 2) optimization of environmental utility and durability (e.g., wear, corrosion-, and oxidation-resistance); 3)

attainment of special properties or combinations of properties (e.g., special electrical, optical, magnetic or thermal properties with strength); 4) minimization of weight; 5) minimization of raw material costs and conservation of limited material resources; 6) ease of fabrication; 7) minimization of fabrication and life-cycle costs; and, increasingly, 8) consideration of environmental compatibility (Refs. 3, 4).

Joining dissimilar combinations of oxide and nonoxide ceramics, intermetallics, glasses, and heat-resistant or refractory metals and alloys, whether in monolithic or reinforced forms, poses particular challenges (Refs. 2, 3, 5). Drastic differences in atomic structure, chemical composition, and physical or mechanical properties between different material types cause serious problems of incompatibility that prevent direct joining by fusion welding and, often, by non-fusion welding relying on plastic deformation, and pose challenges even to indirect methods employing heterogeneous filler materials (e.g., brazing or soldering) (Ref. 3).

Joining techniques using functionally gradient materials or FGM joints bridge incompatibilities in chemistry and properties by changing composition from one joint element to the other. Composition changes can be accomplished in steps using discrete layers or continuously by blending materials from a composition that is compatible with (even if not identical to) one end element to a composition that is compatible with (even if not identical to) the other end element. In either case, property differences or mis-

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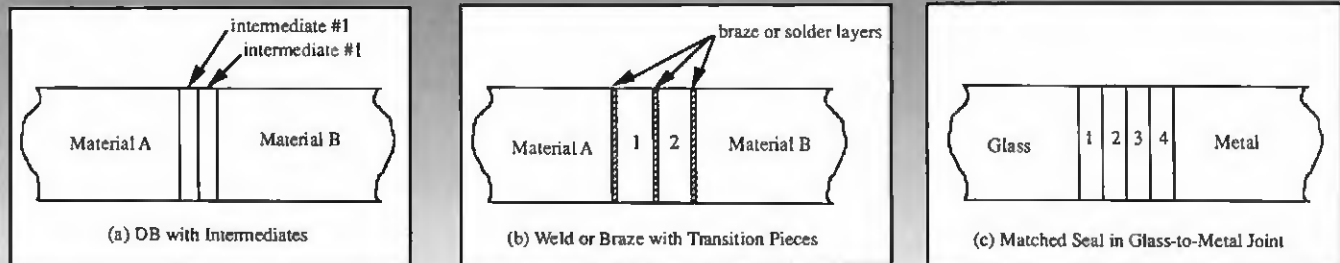


Fig. 1 — Schematic of stepped functionally gradient material (FGM) joints in: A — diffusion brazing/welding using single or multiple intermediates or interlayers; B — welded, brazed or soldered joints using multiple layers or transition pieces; C — multiple transition pieces used in producing "matched seals" between glasses or between a glass and a metal.

matches that would otherwise preclude atomic bonding or lead to bond failure through mismatch stresses are avoided or, at least, are lessened.

The use of discrete layers for joining is not new. Single or multiple interlayers are commonly used in solid-state diffusion welding (Refs. 7, 8), multiple layers or transition pieces are commonly used in "sandwich" brazing and in soldering of dissimilar metals or alloys (Refs. 9–11), of metals to ceramics or glasses (Ref. 2), or even of different glasses in so-called "matched seals" (Ref. 12). While such intermediates can perform many functions, the most important is almost always to gradually change the coefficient of thermal expansion across the joint to preclude development of destructively high stresses. Examples of the use of such stepped FGMs are shown in Fig. 1.

The use of continuous functionally gradient materials for joining is rather new, as, in the past, they could not be easily accomplished due to lack of suitable processing options (e.g., plasma spraying, chemical or physical vapor deposition).

Self-propagating high-temperature synthesis (SHS) offers particular promise as a joining process for many difficult-to-join ceramic or intermetallic materials or dissimilar material combinations (Refs. 13, 14). Briefly, the process involves the reaction of powdered elemental solids, solids and gases, or elements and compounds to produce a new compound or compound and element with the release of substantial exothermic heat of formation. The reaction begins when the mixture reaches a triggering or initiation temperature (T_i), raises the temperature locally at a reaction front through adiabatic heating to a combustion temperature (T_c), and the reaction progresses spontaneously using the heat of formation to drive the reaction front.

The process is attractive for joining for several reasons, including: 1) capability for generating high temperatures to enable atomic bonding through localized melting and wetting of substrates or

through solid-state reactions or interdiffusion with substrates; 2) minimal heat effect in substrates due to the speed of the reaction and the highly localized nature of heating caused by the reaction; 3) high-energy efficiency (with the majority of heat needed for joining being generated internal to the process); 4) facility for production of functionally gradient material (FGM) joints; 5) ability to incorporate reinforcing phases in the filler material (for joining composites or producing composite filler materials *in situ*); and 6), and not incidentally, essentially the same process for joining as was used or could have been used to produce the joint end elements in the first place (Refs. 15, 16). Beyond these advantages, SHS has potential for joining as either a primary or secondary process, where in primary joining end elements are joined at the time they are, themselves, being synthesized and where in secondary joining preexisting joint components are joined as in classic welding and brazing.

As promising as SHS is for producing FGM joints between dissimilar materials, processing engineers engaged in research and development, and often in production, need to design these joints to overcome process-induced stresses from mismatch of coefficients of thermal expansion (CTE) between end-elements and/or intermediates. Likewise for the fabrication of discrete FGM joints by other processes. Such "cured-in" stresses arise during joint fabrication due to the wide excursion in temperature between the temperature at which the joint is produced and room temperature. If too high, they can cause adhesive failure at interfaces or cohesive failure immediately adjacent to interfaces in weak-boundary layers. Thermally induced stresses can also arise in service from excursions of temperature and/or gradients in temperature associated with operation, but these are routinely dealt with rigorously by structural designers.

While other critical design requirements of FGM joints are that they bridge chemical incompatibilities between end

elements, provide required mechanical properties in the joint (e.g., strength, modulus, or toughness, as required), and exhibit microstructural stability under service temperatures, coefficient of thermal expansion (CTE) mismatch is most important during joint formation.

Objective

The objective of the work presented here was to develop a simple model for assisting with the design of functionally gradient material joints consisting of discrete steps or layers between dissimilar end elements. The model was to be capable of predicting the temperature distribution and associated thermally induced stresses in such joints for a wide variety of materials, and to facilitate design to reduce cured-in stresses associated with joint fabrication, regardless of the process employed.

Description of Model

Heat Transfer Analysis and Temperature Distributions in FGM Joints

The basic differential equation of heat conduction for a three-dimensional Cartesian coordinate system is:

$$\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + \dot{q} = \rho C_v \frac{\partial T}{\partial t} \quad (1)$$

where x , y and z are the three Cartesian directions, k is the thermal conductivity, ρ is the density, C_v is the volume specific heat, and \dot{q} is the value of any internally generated heat. To determine the heat distribution in a typical FGM joint during cooling following processing (or under the influence of an imposed operating temperature gradient), one can consider the joint to be a simple planar slab with constant surface area, ends at prescribed boundary temperatures of T_1 and T_2 , and with no internal heat generation, so the problem reduces to a case of one-di-

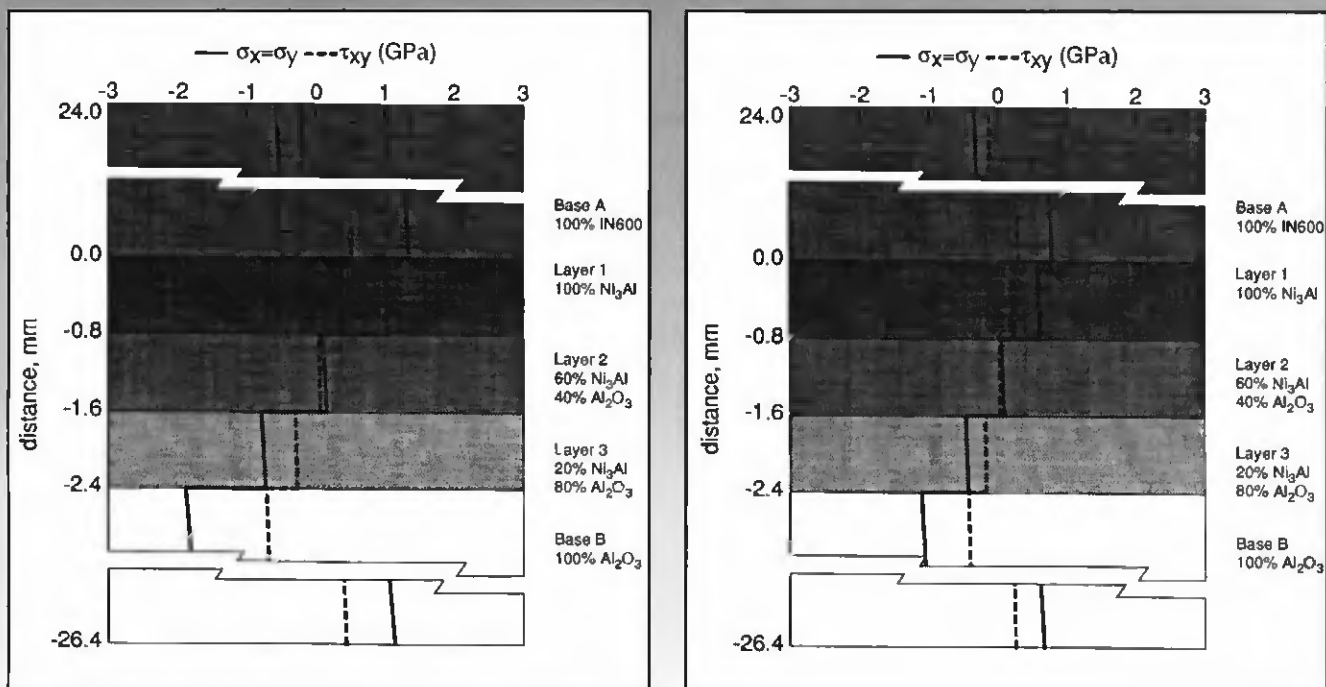


Fig. 3 — Predicted cured-in stresses for two different simulated processing cycles. A — 1500 to 300 K; B — 1000 to 300 K.

$$[A_i] = \sum_{i=1}^n [Q_i](h_i - h_{i-1}) \quad (8a)$$

$$[B_i] = \frac{1}{2} \sum_{i=1}^n [Q_i](h_i^2 - h_{i-1}^2) \quad (8b)$$

$$[D_i] = \frac{1}{3} \sum_{i=1}^n [Q_i](h_i^3 - h_{i-1}^3) \quad (8c)$$

The thermal forces in a layer are produced by the constraints placed on its free deformation by adjacent layers. Because the coefficient of thermal expansion of an individual layer and its adjacent layers are different, a temperature change (or difference) will result in unequal thermal strains so thermal moments are induced. The thermal forces and moments can be obtained by

$$\begin{bmatrix} N_x^T \\ N_y^T \\ N_{xy}^T \end{bmatrix} = \Delta T \times \sum_{i=1}^n [Q_i] \alpha_i (h_i - h_{i-1}) \quad (9)$$

and

$$\begin{bmatrix} M_x^T \\ M_y^T \\ M_{xy}^T \end{bmatrix} = \frac{1}{2} \Delta T \times \sum_{i=1}^n [Q_i] \alpha_i (h_i - h_{i-1}) \quad (10)$$

where h_i and h_{i-1} define the position of a layer in a multilayered material — Fig. 2.

From the above analysis, it is clear that the magnitude of induced thermal stresses depends on the thickness of in-

dividual layers, the number of layers, the temperature change or prevailing gradients, and material properties (α , k , E , G and ν) as functions of temperature. In order to reduce cured-in stresses from fabrication processes and residual stresses arising during service, a computer program has been developed to analyze the relationship between thermal stresses and joint design parameters. The source code for computing temperature distribution and thermal stresses was developed using FORTRAN computer language on an IBM ES/9000 Model 580 large-scale computer using the MTS (Michigan Terminal System) operating system. This source code can be transferred to any computer system (e.g., Macintosh, IBM PC, etc.) provided a FORTRAN compiler is available.

Results Obtained for Typical Cases

The true test of the utility of a model is its ability to predict outcomes for meaningful situations or cases. Ultimately, predictions should be verified by experimental measurements (e.g., here, residual stresses using neutron diffraction). Initially, however, a test of the validity and utility of a model's predictive capability can be seen from whether it allows cured-in stresses to be reduced to permit successful joint fabrication. Also, predictions of the model can be used to identify general effects of joint design changes on process-induced stresses.

To assess and demonstrate the utility

of the analytical thin-plate layer model described here, the results obtained for several cases representative of the variety of situations and conditions that must be dealt with during the production of FGM joints by SHS or other joining processes are presented below. The relationship of each case to general joining is emphasized, where appropriate.

For illustration here, in each case the joint consists of a ductile, nickel-based alloy (Alloy 600) end element (with a nominal CTE of $14 \times 10^{-6} \text{ K}^{-1}$) joined to a brittle, alumina ceramic (Al_2O_3) end element (with nominal CTE of $6 \times 10^{-6} \text{ K}^{-1}$) using multiple steps or layers of gamma (γ) nickel aluminide (Ni_3Al) (with nominal CTE of $12 \times 10^{-6} \text{ K}^{-1}$) mixed with various volume fractions of alumina (Al_2O_3) particles. Overall joint processing temperatures and individual end-element operating temperatures were varied to produce different cured-in or service-induced residual stresses. Joint end elements were taken to be either circular or square in cross-section to make the normal stresses σ_x and σ_y the same (i.e., $\sigma_x = \sigma_y$). The assembled joint was free to expand or contract in its axial (or longitudinal) direction, making the normal stress σ_z zero. The particular joint material combination is not important to this presentation; what is important is the effect of various design changes on the magnitude of thermally induced normal (σ_x and σ_y) and shear (σ_{xy} or τ_{xy}) stresses.

Before employing the model for more complicated discrete FGM cases, its gen-

