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Review
Modelling studies applied to functionally graded materials

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This review contains a description of modelling studies relative to functionally graded materials (FGMs). Two principal topics are covered: models for microstructure-dependent thermophysical properties, and models for the design, processing, and performance of FGMs. The former is a particularly important input to FGM modelling because of the wide variety of microstructures that can exist across the graded direction of a single material. Based on the work described in this review, recommendations are made regarding areas in which additional modelling studies would be beneficial. Suggested approaches to the modelling include the application of a number of powerful techniques, such as percolation theory, fractal analysis, lattice-based microstructure models, the renormalization group, neural networks, and fuzzy logic.

1. Introduction

A functionally graded material (FGM) is a composite, consisting of two or more phases, which is fabricated such that its composition varies in some spatial direction. This design is intended to take advantage of certain desirable features of each of the constituent phases. For example, if the FGM is to be used to separate regions of high and low temperature, it may consist of pure ceramic, at the hotter end, because of the ceramic's better resistance to the higher temperatures. In contrast, the cooler end may be pure metal because of its better mechanical and heat-transfer properties.

A major problem in the design of an FGM, aside from that of materials selection, lies in determining the optimum spatial dependence for the composition. This can be regarded as that composition profile which best accomplishes the intended purpose of the material while maintaining other thermal, physical, and mechanical properties within limits that ensure acceptable performance. Another problem lies in predicting the characteristics of an FGM, for a given composition profile, during fabrication and under in-service conditions. Use of theoretical models to aid in FGM design and to predict FGM fabrication and in-service behaviour is of crucial importance. Once established, a model can readily be used to conduct a wide variety of computer "experiments" in which effects of changing input parameters, such as thermophysical properties of the constituent phases, or the composition profile along the graded direction, are systematically evaluated.

The fact that the composition of an FGM can vary over such a wide range means that a variety of fundamentally different microstructures can exist across the graded direction. This, in turn, means that the thermophysical properties, which are generally strongly dependent on the microstructure, will also vary with position within the material. A realistic model must appropriately account for this fact.

This review includes two aspects of the modelling procedure. First, we consider approaches to calculating microstructure-dependent thermophysical properties. This particular subject is one which has been extensively developed, over the years, so our considerations here are limited principally to applications related to FGMs. Attention is then turned to the models themselves, emphasizing approaches used to date for analysis of materials design, fabrication, and performance. Models for design and performance are not considered separately, because FGM design cannot be carried out apart from consideration of in-service conditions. Likewise, performance modelling would yield vitally important information to be fed back for design modification. Finally, based on existing work, attention is directed to areas in which additional modelling is still required, and recommendations along these lines are made.

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2. Models for thermophysical properties

2.1. General comments

The problem of calculating effective thermophysical properties of heterogeneous materials is an old one, dating back to Maxwell [1] and Rayleigh [2]. However, with new applications for such materials continuing to emerge, interest and activity in this subject continues to the present day. New approaches are sometimes developed with specific applications in mind (e.g. to electrical, magnetic, superconducting, mechanical, or thermal properties), and, consequently, are therefore not made readily accessible to all who might be interested. This is unfortunate, because their applicability may extend well beyond their immediately intended use. Some particularly comprehensive reviews, related to this general subject, have been published within the past several years, i.e. by Torquato [3], Bergman and Stroud [4], and Nan [5].

As already has been noted, the effective thermophysical properties of heterogeneous materials are intimately related to the microstructure of the material. Along these lines, Nan [5] has identified three basic types of geometric morphologies associated with the distribution of phases within a two-phase material.

(i) *Dispersed grain structure.* This is characteristic of a material for which the volume fraction of one phase is low, and is discretely and randomly distributed within the host phase (Fig. 1a). It is also characteristic of a material for which the volume fraction of the dispersed phase is somewhat higher, but the phase remains discretely and uniformly dispersed (Fig. 1b).

(ii) *Aggregated grain structure.* This morphology characterizes the case for which the volume fraction of the minor phase is increased to the point that it is no longer discrete, but is aggregated in the form of clusters of definite size (Fig. 1c).

(iii) *Percolation-like cluster structure.* As the volume fraction of the minor phase is increased still further, it reaches a critical value, called the percolation threshold, at which it is interconnected to such an extent that there exists a continuous random cluster, as well as smaller aggregated clusters (Fig. 1d).

These qualitative definitions are quite helpful. However, we do need to have *quantitative* descriptions as well, that can, in turn, be related to the description of effective thermophysical properties. Likewise, we need to be able quantitatively to describe the transition from one microstructure to another as the composition varies.

A great deal of effort has been devoted, over the years, to the development of thermophysical-property models for a dilute, discrete dispersion of one phase within another. However, the case of intertwined networks of the two phases, as illustrated in Fig. 1d, presents particularly interesting behaviour. If, for example, the electrical conductivity of one phase is significantly higher than that of the other, then a sharp increase in the effective electrical conductivity of the mixture would take place at the composition for which the relative amount of the higher-conductivity component reaches its percolation-threshold value. A schematic illustration of this behaviour is given in Fig. 2. Indeed, a variety of topological features of the microstructure need to be considered in order to develop physically realistic property models. These include directionality, connectivity, and irregularity of the phases that are present.

The description of these complex microstructures can involve some unusual difficulties, one example being the case of percolation. Chernikov and Rogalsky [6], have pointed out that studies in two-dimensional percolation theory, have, over this past decade, borne considerable fruit. However, the three-dimensional problem presents greater difficulties, there still being no exact analytical treatments for lattice percolation and random continuum percolation, although numerical studies have been carried out.

A question that must also be addressed is that of how much information regarding microstructure must be included in order to describe adequately material properties and behaviour. This particular issue was recently treated by Becker and Richmond [7], as it

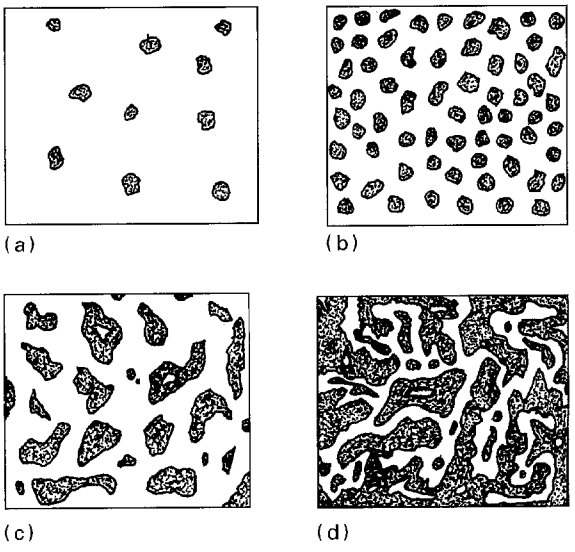

Figure 1 Illustration of the basic types of microstructures for a two-phase heterogeneous material, as proposed by Nan [5]: (a) randomly dispersed structure; (b) uniformly dispersed structure; (c) aggregated structure; and (d) percolation-like structure.

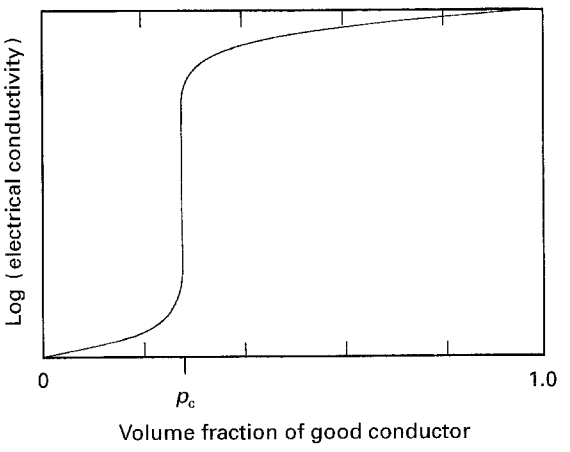

Figure 2 Schematic illustration of the variation with composition of the electrical conductivity of a two-phase mixture, one phase being a good conductor, the other a poor conductor. The quantity p_c is the percolation threshold.

relates to effects of grains, pores, and second-phase particles in numerical simulations of the mechanical response of ductile materials. Their models were limited to two dimensions, although the need for inclusion of microstructural features, in order to be physically realistic, was demonstrated.

2.2. Application to FGMs

The manner in which the microstructure might vary across an FGM is shown schematically in Fig. 3. This particular material is shown as consisting of one pure component at one end, then developing a discrete dispersion of a second component further along the graded direction. Still further along this direction, the mixture consists of two complex, intertwined networks of the two components. Then, nearer to the other end of the FGM, the mixture again becomes a discrete distribution, now of the first component within the second. Finally, the material is pure again, consisting of the second component alone. Clearly, these are major microstructural variations, which must be appropriately accounted for in terms of thermophysical-property models and in terms of response of the material to its environment (thermal, mechanical, electrical, magnetic, etc.).

The uniqueness of this problem, as applied to FGMs, has led to its being the subject of several recently reported studies. For example, the topological changes that occur along the gradient direction of a metal/ceramic FGM (stainless steel and partially stabilized zirconia) were analysed by Muramatsu *et al.* [8]. Near one end of the material, the microstructure consisted of discrete ceramic particles dispersed within a metal matrix. Conversely, the region near the other end contained discrete metal particles dispersed within a ceramic matrix. However, the transitional region between these two extremes contained a network structure in which each of the two constituents existed as an interconnected phase; thus, the question of the extent of connectivity or percolation became important (in the sense of the above discussion centred around Fig. 2). A quantitative study of the microstructural transition was carried out using techniques of fractal analysis. Specifically, a method of "mass fractal analysis" was used for the network structures and "surface fractal analysis" for the discretely dispersed structures. The analyses were found to be particularly useful for quantitatively describing the gradual transition from one structure to another (e.g. network to discrete) as a function of the volume fraction of metal or ceramic. Their results also correlated well with experiment: as the metal content of a metal/ceramic mixture decreased, passing through a transition from a network to a dispersive structure (as measured by the variation of a fractal dimension), a sharp reduction in the electrical conductivity of the mixture was found to occur.

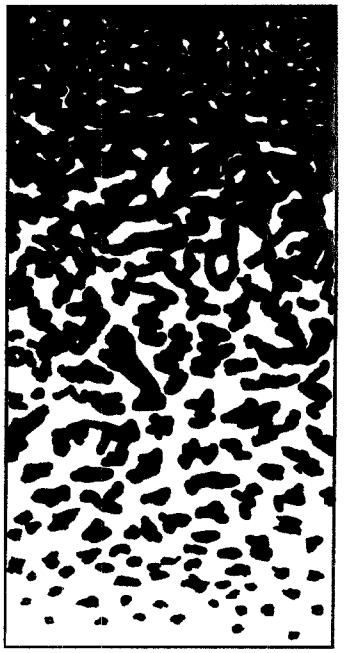

Figure 3 Schematic illustration of the microstructure of a two-component FGM, for which the composition gradually varies from entirely the one component to entirely the other.

A similar approach was used by Zhang *et al.* [9] for describing topological features of FGMs. They used percolation theory to describe the transition from a discretely dispersed second phase to a network structure. They also used fractal geometry to describe the irregularity associated with particle clusters within the material.

Models for specific thermophysical properties of a heterogeneous material are based on some kind of microstructure-dependent "mixture rule". Although such rules have long been used to at least semi-quantitatively describe the properties of such materials, their development, for one application or another, continues to the present. For example, Fan *et al.* [10] have derived a generalized law of mixtures for use in predicting the mechanical properties of two-phase composites (phases A and B). This law, which is applicable to a number of mechanical properties, can be applied to any volume fraction, grain shape, or phase distribution, and has been shown to yield excellent agreement with experimental data. It accounts for contributions to the overall mechanical properties of a composite as arising from three sources: the pure phases, A and B, and an A–B mixture.

Another example of the use of mixture rules is represented in the work of Wakashima *et al.* [11], which is discussed here in some detail specifically because of its application to the modelling of FGMs. They considered a material having two components, again denoted as A and B. Let P_A and P_B be the values of some particular property for pure A and pure B, respectively, and let their respective volume fractions be f_A and f_B, where $f_B = 1 - f_A$ if the material is 100% dense. For an FGM, these fs are dependent upon position along the graded direction. The well-known Voigt-type estimate for the effective value, P, of this property is

$$P = f_A P_A + f_B P_B \quad (1)$$

which is simply an arithmetic mean. On the other hand, the likewise well-known Reuss-type estimate is

given by

$$\frac{1}{P} = \frac{f_A}{P_A} + \frac{f_B}{P_B} \quad (2)$$

which is a harmonic mean. As the authors pointed out, these expressions have only limited validity. They discussed the use of a more general expression

$$P = f_A P_A + f_B P_B + f_A f_B Q_{AB} \quad (3)$$

where Q_{AB} is a function that depends on P_A, P_B, f_A and f_B, as well as on microstructure-dependent quantities. The functional form for Q_{AB} was given for four properties (thermal conductivity, coefficient of thermal expansion, bulk modulus, and shear modulus) for the case in which the microstructure consists of spherical particles of constituent B embedded in a host phase, A. Consider, for example, their expression for thermal conductivity, which is given by

$$\lambda = f_A \lambda_A + f_B \lambda_B + f_A f_B \frac{\lambda_A - \lambda_B}{\{3/[(\lambda_B/\lambda_A) - 1]\} + f_A} \quad (4)$$

where λ_A and λ_B are the thermal conductivities of pure A and pure B, respectively, and λ is the effective thermal conductivity of the mixture.

Equation 4 can be compared with analogous results obtained by other investigators. For example, Christensen [12] derived such an expression (his Equation 2.13) based on effective-medium theory. With this approach, which is illustrated in Fig. 4, he considered the details of the temperature distribution within and immediately outside a single-phase-B inclusion. The remaining material, extending to infinity, was treated as being effectively homogeneous. His result is mathematically equivalent to Equation 4. The effective-medium approach, at least in the sense of considering contributions from pure phase A, pure phase B, and an A–B mixture, has some analogy with the work of Fan *et al.* [10].

We now determine the extent to which properties calculated from Equations 1–3 differ from one another. To illustrate this comparison, we again consider the thermal conductivity, using Equation 4 as the more general expression. In Fig. 5, the thermal conductivity is plotted as a function of composition for all three approximations for selected values of the ratio λ_A/λ_B. The abscissa covers the entire range,

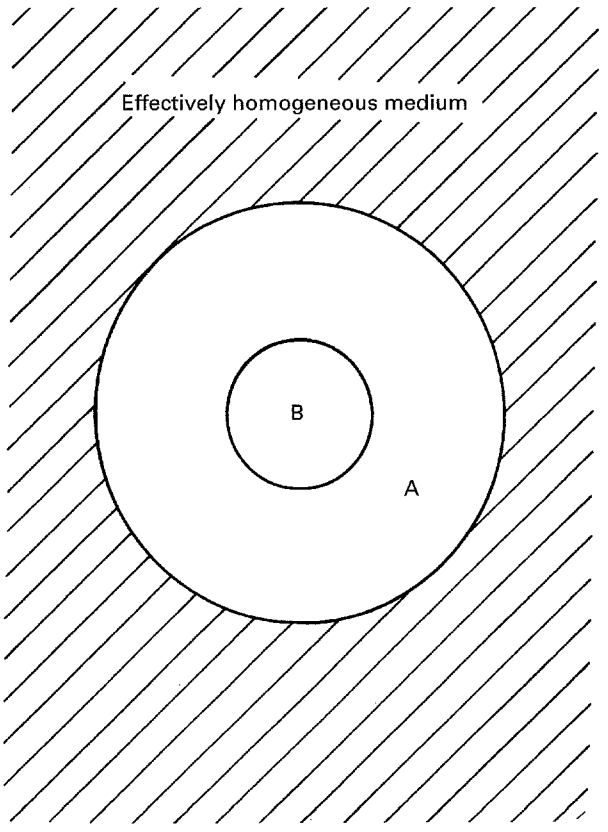

Figure 4 Effective-medium approach to calculating properties of a discrete distribution of minor phase, B, within host phase, A.

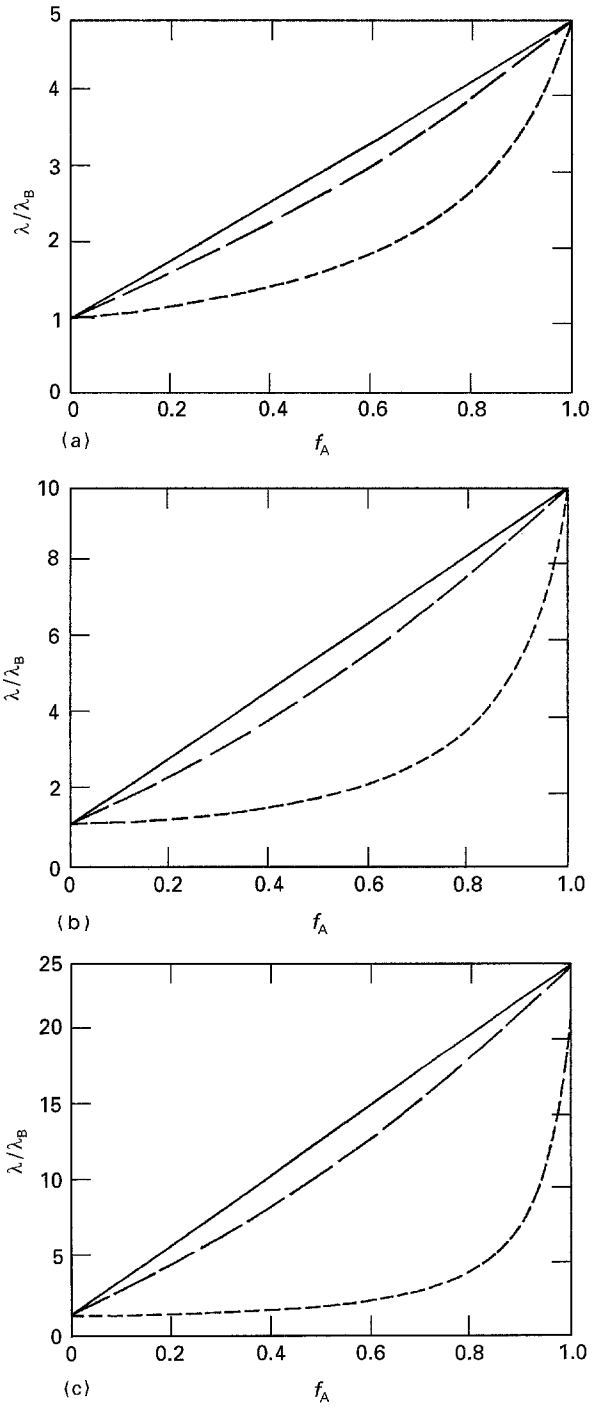

Figure 5 Variation of effective thermal conductivity, λ, with volume fraction, f_A, of phase A. (——) Arithmetic mean (Equation 1); (- - - -) harmonic mean (Equation 2); (— — —) the more general result (Equation 4). λ_A/λ_B = (a) 5, (b) 10, and (c) 25.

$0 \leqslant f_A \leqslant 1$, although the assumption of dispersed spherical phase-B particles is clearly not valid for the smaller values of f_A. From this figure, we make the following observations. First, the more general approximation, as expected, lies between the Voigt-type and the Reuss-type averages. Second, the Voigt-type average is surprisingly close to the more general case for all compositions and for all indicated values of the ratio λ_A/λ_B, with the difference between the two tending to increase as this ratio increases.

Additional considerations of mixture rules for thermophysical properties were given by Hirano *et al.* [13], who related the pertinent rule for various properties (thermal conductivity, coefficient of thermal expansion, elastic modulus and shear modulus) to the nature of the microstructure. The specific microstructures they included were laminates, fibre composites with fibres aligned transversely and longitudinally to the gradient direction, thin-layered composites, and composites in which the second phases are either flake-like or spherical inclusions.

Another way to estimate properties of heterogeneous media is to use statistical information on the microstructure to compute rigorous bounds on property values. These methods were recently reviewed by Torquato [3], who showed that these bounds can often be used to provide good estimates of properties despite having incomplete statistical information on the microstructure. In some cases, these methods can result in improved predictions over bounds computed solely from the volume fraction occupied by the constituent phases and from individual phase properties.

Still another approach to describing transport properties in heterogeneous media is that developed by Ben-Amoz [14], in which the concept of heat transfer, as a whole, is re-developed starting with an analysis of "micro- (or local) conduction" within a "micro-medium". The collection of all these micro-media makes up the entire medium. The macroscopic heat-conduction equation, and the pertinent boundary conditions, are obtained using a variational formalism. This approach was extended by Baker-Jarvis and Inguva [15] using Green function techniques. In addition, an approach analogous to that used by Ben-Amoz [14] was used by the same author [16] to develop a theory for the dynamical behaviour of composite materials; here, a system of equations was obtained for the macro-motion within a medium having arbitrary phase geometry.

Analytical and numerical models for mechanical and thermal properties of plasma-sprayed ceramic coatings were recently described by Argyris *et al.* [17] as a function of the microstructure. Although these studies were not directed specifically toward FGMs, they are nevertheless relevant from the standpoint that plasma spray is one method for fabrication of FGMs. In addition, they pointed out that data for certain thermal properties of sintered ceramics differ from those for ceramics prepared by plasma spraying. Mechanical behaviour was studied using a computer-generated microstructure of a lamellar ceramic coating. Thermal conductivity was calculated as affected by the presence of pores described by ellipsoids of revolution. Of the geometrical factors considered, i.e. pore volume, orientation, and aspect ratio, the volume was most significant in terms of reducing the effective thermal conductivity.

Experimental measurement of properties is, of course, also of great importance. For example, Kumakawa *et al.* [18] studied thermomechanical properties of FGMs under conditions of large temperature difference. Steady-state thermal exposure tests were conducted to determine thermal-fatigue properties. The conclusion was that material deterioration caused by thermal cycling can be estimated by assessing the concomitant degradation of its effective thermal conductivity, even to the point of predicting thermal-fatigue life. Moreover, FGM specimens exhibited better thermal resistance and longer thermal-fatigue life than "conventional" materials, indicating that FGMs are indeed promising materials for these applications. Other studies have also found that use of FGMs results in performance that is superior to that obtained when non-graded materials are used.

3. Models for functionally graded materials

In this section, we review approaches that have been used for modelling FGM design, processing, and performance. We look first at models for the spatial variation of composition, then at systems-type models for design and performance, and finally at models developed for a variety of aspects of FGM behaviour. Again, we emphasize the fact that processing and performance are integrally connected (reflected by the fact that features of both have been incorporated into various models).

3.1. Models for spatial variation of composition

FGM models generally require an assumption regarding the spatial distribution of their constituent phases. Consider, for example, an FGM that has two constituents, which we denote as 1 and 2. Assume the geometry is one-dimensional, with the x-direction being the direction of the microstructural gradient. We first treat the local volume fraction of phase 1, $f_1(x)$, as a continuous function (the volume fraction of phase 2 being $1 - f_1(x)$ if the material is fully dense). These functions can be quite simple, the ability to exhibit curvature, both "concave upward" and "concave downward", being desirable. One example that is used is after Wakashima *et al.* [11]

$$f_1(x) = \left[\frac{x_2 - x}{x_2 - x_1}\right]^N \tag{5}$$

where x_1 and x_2 border regions of pure phase 1 and phase 2, respectively, and N is a variable parameter, the magnitude of which determines the curvature of $f_1(x)$. This function is illustrated in Fig. 6 for selected values of N. It can be seen that the curvature can be made concave upward and concave downward, to a greater or lesser degree, by proper choice of N.

Essentially the same functional dependence was also used by Watanabe and Kawasaki [19, 20], Hülsmann and Bunk [21], and Kuwahara *et al.* [22]. A quadratic function was used by Markworth and Saunders [23], i.e.

$$f_1(x) = a_0 + a_1 x + a_2 x^2 \quad (6)$$

where the as are variable parameters whose values are determined by imposed constraints and by the optimization process itself. These simple functions still offer considerable flexibility of choice relative to the "shape" of the $f_1(x)$ function.

Equation 6 is plotted in Fig. 7 for the case in which $f_1(0) = 0$ and $f_1(l) = 1$, where l is the FGM thickness along the graded (i.e. the x-) direction. These two conditions can be used to eliminate a_0 and a_1 from Equation 6, leaving a_2 as the sole variable parameter. The two curves shown represent maximum and minimum allowable values for a_2 (l^{-2} and $-l^{-2}$, respectively) to ensure that f_1 does not fall below zero or exceed 1 within the range $0 < x < l$. Comparing Figs 6 and 7, it can be seen that Equation 5 offers a greater range of composition profiles than does Equation 6, although the latter equation can be shown to be simpler to deal with, from an analytical point of view, than the former.

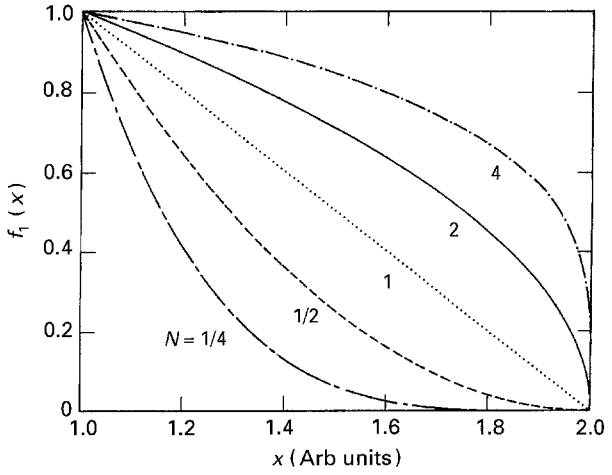

Figure 6 Plot of $f_1(x)$ versus x (Equation 5), for selected values of N, with $x_1 = 1$ and $x_2 = 2$.

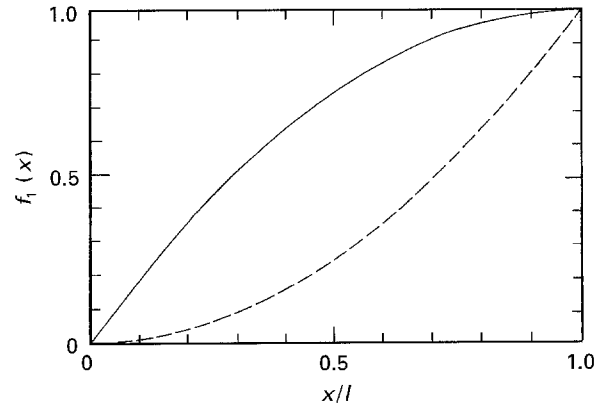

Figure 7 Plot of $f_1(x)$ versus x (Equation 6) for (———) minimum a_2 and (– – –) maximum a_2, taking $f_1(0) = 0$ and $f_1(l) = 1$.

A more elegant approach to FGM design is that used by Tanaka *et al.* [24, 25], who used direct sensitivity and optimization methods to adjust the composition profile and thereby reduce thermal stresses. The profile change, taking place during one optimization process, is illustrated in Fig. 8 [25] for an Al–SiC FGM. To design the composition profile [25], they used composition-dependent thermophysical properties based on a theory of spherical inclusions, together with an interpolation, based on a "fuzzy inference", the latter having been used within the composition range $0.3 \leqslant f_1(x) \leqslant 0.7$.

Another approach to modelling the spatial variation of composition would be to select $f_1(x)$ such that it changes discontinuously, in a finite number of steps, across the graded direction. This would be appropriate for describing an FGM that is fabricated by bonding together several layers of material that differ in composition from one to the next.

Of course, from knowledge of $f_1(x)$, and from other knowledge regarding the composition-dependent microstructure, one can determine the corresponding x-dependence of effective values to be used for thermophysical properties, such as the thermal conductivity, $\lambda(x)$, Young's modulus, $E(x)$, and coefficient of thermal expansion, $\alpha(x)$. These, in turn, can be used to calculate temperature and stress distributions. The temperature distribution, $T(x)$, is determined, under steady-state conditions from

$$\lambda(x)\frac{dT}{dx}(x) = \text{constant} \quad (7)$$

the solution of which is subject to appropriate boundary conditions. The normal stress distribution, $\sigma(x)$, is given by

$$\sigma(x) = -\kappa\alpha(x)E(x)[T(x) - T_c] \quad (8)$$

where T_c is the temperature at the cooler end of the FGM and κ is a constant equal to 1 for plane stress and $(1 - \nu)^{-1}$ for plane strain, where ν is Poisson's ratio. Of course, one can also calculate the associated strain field, as was done by Wakashima *et al.* [11].

These basic illustrations demonstrate the linkage that exists between FGM design and performance.

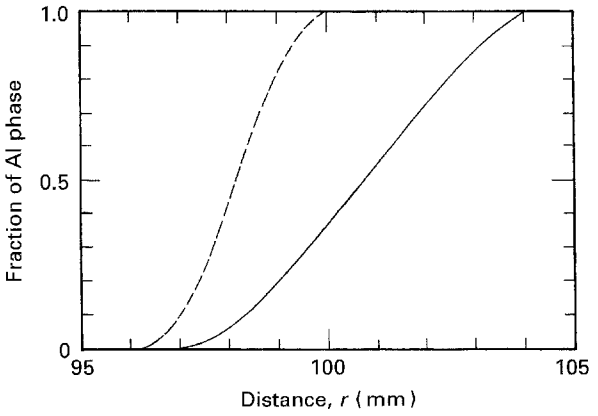

Figure 8 Optimization of composition profile for an Al–SiC FGM, as calculated by Tanaka *et al.* [25] (after their Fig. 6). (– – –) The initial profile, (———) the optimized profile.

Determination of $f_1(x)$ is related to design, whereas calculation of $T(x)$ and $\sigma(x)$ is related to performance, and in addition, to fabrication [19]. However, calculation of $T(x)$ and $\sigma(x)$ may indicate a need to revise the current $f_1(x)$ if, for example, the thermal stress is predicted to reach excessively high values.

3.2. Systems approach to FGM modelling

A useful approach to the overall modelling of FGM processing is based on a systems-analysis strategy, that has been used by various investigators (see, for example [9, 11, 13, 19, 26]). For example, an "inverse design procedure" has been developed [13, 26] and is illustrated by the flow chart shown in Fig. 9. Here, the structure and the boundary conditions are specified initially. Then, several combinations of materials are assumed along with different assumptions for the spatially dependent mixture ratio. The temperature and thermal stress distributions are calculated for these various combinations, and the calculations are repeated until "optimum" conditions are obtained. Attention is paid, of course, to the use of appropriate microstructure-dependent material-property models.

Another systems-type approach to the optimization process was used by Tanaka *et al.* [24], and consists of the following sequence of steps:

1. choose an initial composition profile;
2. carry out a preliminary analysis of non-stationary heat conduction and thermal stress;
3. at each time step, examine the design (failure) criteria;
4. if the design criteria are violated, calculate a quantity known as the "thermal stress sensitivity increment";
5. find the optimum composition profile that satisfies the design criteria;
6. repeat the analysis of non-stationary heat conduction and thermal stress with the composition profile determined;
7. if the design criteria are violated at another time step, return to Step 4.

These systems-type approaches to FGM design are just ordered sequences of steps, carried out to ensure that the resultant material will perform adequately in its intended application. However, it is important to note that the term "optimum conditions" used above may not necessarily have a unique definition, but may instead involve a set of compromises among various quantities (e.g. material types, heat-flow rate, FGM thickness, maximum thermal stress, etc.) in order that the desired application is achieved over an acceptably long in-service lifetime.

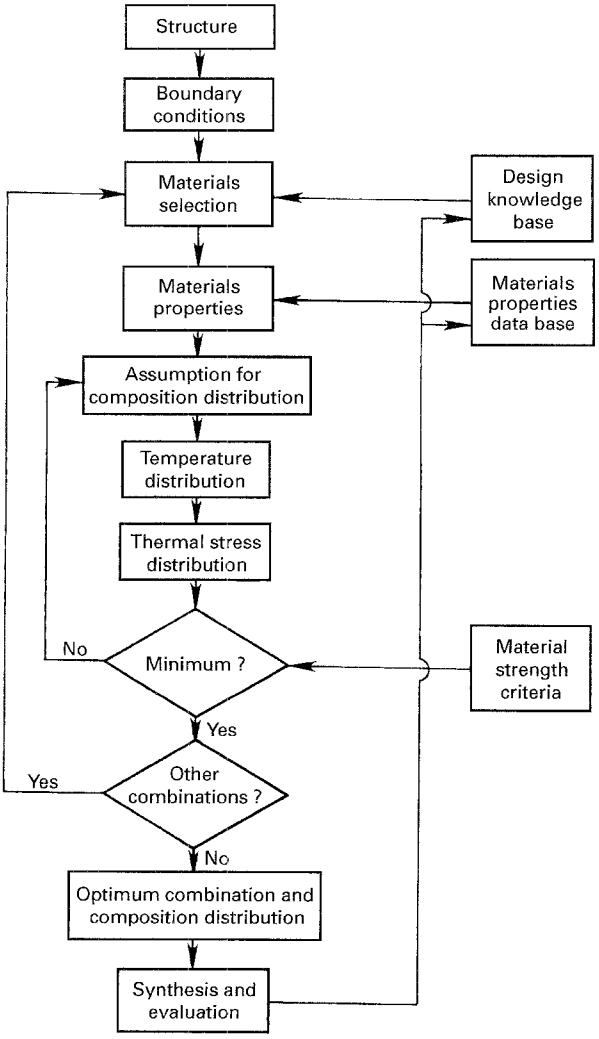

Figure 9 Flow chart for the "inverse design procedure" used for FGM design [13, 26].

3.3. Other studies of FGM behaviour

Next, we turn our attention to some modelling studies that were directed toward a variety of aspects of FGM behaviour. These may vary in degree of sophistication, but they share, together with the studies already described, the common goal of maintaining both the performance characteristics of the FGM and its structural integrity.

An early version of an FGM was studied by Stewart *et al.* [27] for intended use as a thermal protection system for spacecraft re-entry. The anticipated need was for high-temperature capability at one end and good mechanical behaviour at the other end. Two different materials were bonded together to serve this purpose. Computation of thermal response agreed well with experiment. Here is one example for which $f_1(x)$ has two values, one for each of the two materials, and changes discontinuously at the interface between the two.

Work in China [9] is being directed toward a number of mechanical and thermal aspects of FGMs. Included here is an elastic and inelastic micromechanics theory intended to study effective inelastic properties in metal-rich regions where the ductile metal is plastically deformed. Also, a coupled thermoelastic model is being developed to study thermal-shock response of a metal/ceramic FGM caused by abrupt heating.

The simple Markworth–Saunders model [23], described above, was used to maximize or minimize, as desired, the heat flux traversing the graded direction. In so doing, they found some unusual behaviour, as follows: they assumed that $\lambda(x)$, $E(x)$, and $\alpha(x)$ were all given by Voigt-type estimates, after Equation 1, for an FGM that was pure ceramic at one end and pure

metal at the other end ($x = 0$ and $x = l$, respectively). The ceramic end was taken to be at a higher temperature than the metal end. Then for certain values of λ, E, and α for the pure metal and pure ceramic, and for conditions corresponding to the extreme cases of maximum and minimum rates of heat flow across the graded direction, the thermal stress distributions are as shown in Fig. 10. Clearly, the stress distribution for maximum heat flow has a maximum value that lies *inside* the FGM, a fact that would have to be accounted for in material design. Another result (one that was expected) was that the optimum design for minimum heat flux across the FGM contained minimum metal in the structure, subject to imposed design constraints, and vice versa for maximum heat flux.

Results of finite-element calculations of axial, radial, circumferential, and shear stresses in disc-shaped FGMs were reported by Watanabe and Kawasaki [19]. They pointed out two considerations that are relative to such calculations. One is to minimize the thermal stress caused by cooling from the sintering temperature. The other is to minimize the stress generated during performance, e.g. as a thermal barrier.

Another numerical study of thermal stresses in FGMs, associated with both processing and performance, was conducted by Matsuzaki *et al.* [28]. They concluded that one of the important factors affecting these stresses is the compositional distribution. In addition, they found that the key issue for this particular FGM ($MoSi_2$–SiC/TiAl) is the high thermal stress generated during processing, a problem that requires further attention.

A finite element model, developed by Miller *et al.* [29], was intended to be a guide in both the design and fabrication of an NiAl–Al_2O_3 FGM. The model was used to estimate residual stress as a function of structure of the material. It also included effects of thermal cycling.

Elastoplastic analyses were conducted by Giannakopoulos *et al.* [30] of cyclic thermal response in multi-layered materials. These layers consisted of a metal, a ceramic, and an FGM between the metal and the ceramic. Analytical and finite element methods were both used. It was found that the smooth gradation of composition between metal and ceramic resulted, under thermal cycling conditions, in a reduction of (a) thermal residual stress, (b) accumulation of plastic strain, and (c) stress concentrations at free edges. Parametric information was also obtained relative to effects of the FGM on thermal response of the layered material occurring during processing.

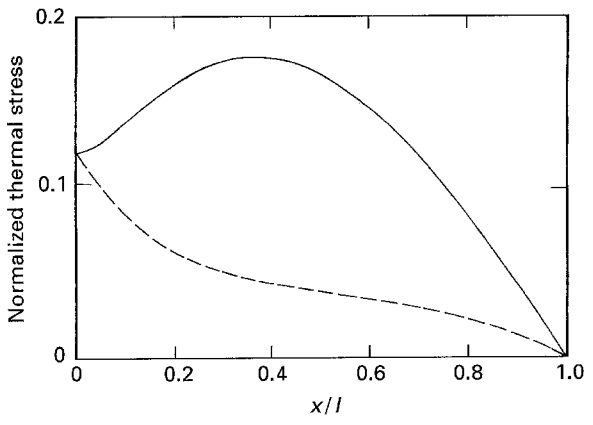

Figure 10 Thermal stress distributions across a metal/ceramic FGM designed for maximum heat flow ((———) corresponding to minimum a_2) and minimum heat flow ((– – –) corresponding to maximum a_2) across the graded direction [23]. The stress is normalized with respect to the maximum thermal stress in an all-metal layer.

A finite element analysis of thermal stresses in metal/ceramic FGMs was carried out by Kawasaki and Watanabe [20] with a 1400 °C temperature difference assumed to exist across the material. A linear dependence of materials properties on composition was assumed. The variables studied were the interlayer width, fineness of the compositional gradation, and the composition profile. They found, for example, that the maximum axial thermal stress decreased strongly with increasing interlayer width. They also calculated this stress as a function of what is our parameter N in Equation 5 above, and found that a value of this parameter exists where the stress is a minimum. In a related study, Matsuzaki *et al.* [31] carried out an analytical design of a ZrO_2/γ-TiAl FGM intended to insulate the cooling structures of Scramjet engines. Use of an FGM having optimized thermal resistance parameters was found to reduce the required mass of coolant to just 35% of that needed for a cooling structure without an FGM.

The thermal shock response to heating abruptly an isotropic metal/ceramic FGM was modelled by Zhang *et al.* [32], who found that thermomechanical coupling exerted a strong effect on this response. One can thus conclude that the neglect of such coupling effects under conditions of non-uniform exposure and sudden, intense heating, needs to be questioned.

Transient thermal stresses in an FGM plate were studied by Teraki *et al.* [33] using an elastic–plastic formalism. A micromechanical approach was used, based on the assumption that local microstructures can be described in terms of spherical ceramic (metal) particles embedded within a metal (ceramic) host phase at volume fractions that vary in a quasi-continuous manner. Transient thermal stresses were calculated for a zirconia/stainless steel FGM plate, subjected to cyclic thermal load, for both elastic and elastoplastic conditions. A possible thermal ratcheting effect was observed.

A study of transient thermal stress intensity factors was carried out by Jin and Noda [34], who modelled a crack in a semi-infinite plate of an FGM. This involved a reduction of the thermal and mechanical problems to two systems of singular integral equations. It was found that substantial lowering of stress intensity factors could be obtained by appropriate selection of thermophysical properties.

Some problems having direct bearing on FGM behaviour were treated by Erdogan and Ozturk [35, 36]. In one of these [35], a mixed boundary value problem was considered that involved processes of heat diffusion and fracture mechanics in a medium consisting of a non-homogeneous layer bonded to a homogeneous substrate, and containing an interface crack. The

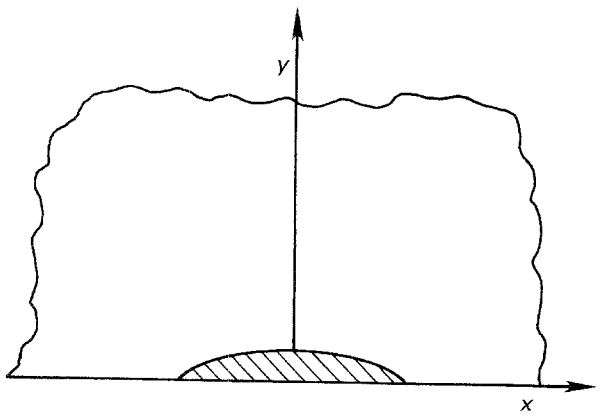

Figure 11 Geometry of the problem treated in [35]. A crack (shaded region) exists at the interface between an inhomogeneous layer bonded to a homogeneous substrate.

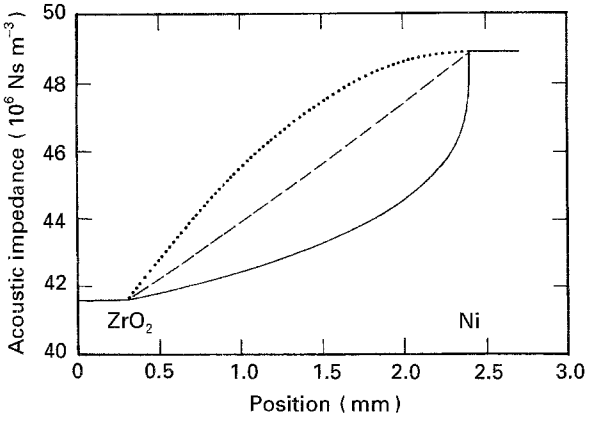

Figure 12 Acoustic impedance profiles calculated for an Ni–ZrO_2 FGM [22], with composition profiles calculated from Equation 5. N = (——) 1/3, (– – –) 1, and (···) 2.

geometry of this problem is illustrated in Fig. 11. In the other [36], consideration was given to the general debonding problem involving homogeneous dissimilar materials bonded through an interfacial region having graded thermomechanical properties.

A non-destructive method for detecting and evaluating the distribution of elastic parameters along the graded direction of an FGM has been developed by Kuwahara *et al.* [22]. The method that was used was "reflection impulse response", which includes determination of the acoustic impedance profile. (Acoustic impedance is the product of density times speed of sound). The composition profile that was assumed is that given by Equation 5. The profile calculated for an Ni–ZrO_2 FGM is shown in Fig. 12 for several values of the parameter N which appears in Equation 5. Good agreement between theory and experiment for the normalized responses, for $N = 1/3$, suggests that the technique is useful as a means with which to evaluate the accuracy of the design.

4. Conclusion

FGMs, still a relatively new technology, appear already to have proven their worth in a variety of applications. Their design presents some unique problems in terms of appropriate models for thermophysical properties and for optimization of structure to achieve certain desired in-service characteristics, including the following [35]: reduction of thermal stress, residual stress and stress concentration factors; improved bonding strength, toughness, and resistance to corrosion and fatigue-crack growth. Modelling these materials is clearly an essential ingredient to attaining successfully these features. Although significant advances in modelling studies have been achieved, in the few years that FGMs have been seriously studied, much remains to be accomplished. The next section contains some recommendations along these lines.

5. Recommendations

On the basis of the work reviewed above, it is evident that significant progress has been made both in calculating thermophysical properties and in actual FGM modelling. Some recommendations relative to areas in which additional work is needed are presented below. In some cases, general approaches to carrying out this work are also suggested.

5.1. Thermophysical-property modelling

1. Techniques such as percolation theory and fractal analysis have already been shown to be extremely important in obtaining a quantitative description of the microstructure of heterogeneous materials, as well as of the variation of microstructure with composition. However, what we need now is to be able to correlate that description with the microstructure-dependent models used to describe thermophysical properties to ensure that the model used, for a given composition, is indeed physically appropriate. This would be a significant improvement over, for example, the use of the same general model covering the entire composition range. Thus, correlations between property models and microstructure need to be studied in greater detail.

2. As a corollary to Point 1, an FGM may indeed cover the entire composition range, e.g. from pure metal at one end to pure ceramic at the other end. Composition-dependent factors discussed earlier, such as directionality, connectivity, and irregularity, will play a major role in affecting the nature of a given thermophysical property and must be considered over the entire composition range. Again, an effort in this direction will lead to property models that are consistent with the local microstructure. Only then can a predictive model for an FGM be used with confidence.

3. Another consideration, relative to thermophysical properties is that the microstructure of an FGM is subject to change during in-service operation. For example, thermal cycling can result in accumulation of damage which in turn, reduces the effective thermal conductivity [18]. Such considerations must be factored into inservice simulations using physical models for FGMs.

4. For certain applications, lattice-based microstructure models may prove to be superior to "effective-property" models. In these models, a two- or

three- dimensional lattice is constructed and each cell is assigned a property corresponding to either of the two materials. Thus, connectivity is directly incorporated into the lattice. The equations describing the phenomena of interest (e.g. heat flow) are then solved directly using the lattice approximation. The general problem is analogous to the Ising problem in ferromagnetics that has received a great deal of attention. An approach, that has been used by Torquato [3] and others, is to solve for the effective properties using the lattice models and then incorporate these properties into an overall continuum model. For some applications, such as ablation of an FGM, the lattice model may be especially attractive, because incorporating the phase change directly into the lattice description may be possible, whereas attempts to use effective properties would be awkward. However, the lattice model becomes difficult when the volume to be modelled becomes large, due to the excessive number of lattice sites required. Retaining the connectivity information offered by the lattice approach, together with the averaging offered by an effective-property model, would be attractive. One method that should be explored is the renormalization group (RNG). In the simplest form of RNG, a lattice is first constructed, and then a coarse lattice is constructed over it. The equations describing the coarse cell are required to be mathematically similar to the fine grid equations when they are rescaled. Ultimately, one obtains a coarse-grid lattice that has retained connectivity information and other characteristics of the fine grid. We are not aware of the application of the RNG to FGMs, but the technique has been used to treat a wide variety of physical phenomena (including the Ising problem) and its applicability to FGM design and performance modelling should be explored.

5.2. Structure optimization, processing, and performance modelling

1. Pursuant to Point 3 of Section 5.1, the accumulation of damage within an FGM may be a life-limiting factor. Given that large temperature differences (around 1000 °C) can exist across the gradient direction, that large differences in thermal expansion may exist between the phases, and that FGMs are subjected to conditions of thermal cycling, it is necessary that service-life-prediction techniques be appropriately adapted to FGMs. Along these lines, failure criteria appropriate specifically to spatially varying microstructures must be developed.

Of course, in this and other areas, modelling studies must both support and be supported by the execution of pertinent experiments. For example, the need for detailed experiments relative to diffusion, microstructural stability, and creep within an FGM, under thermal-fatigue conditions, has been stated [30]. Further needs include critical experiments that would measure constitutive response under uniaxial and multiaxial loading conditions, including conditions for which straining is non-proportional [30].

2. Although the topic of thermal stress generation during FGM processing has already been addressed by a variety of investigators (e.g. [19, 28–30]), the subject is still acknowledged to be of major importance and to require further modelling analysis.

3. Optimization of the FGM structure is a problem of crucial importance, and is complicated because property variations along the gradient can be highly non-linear or discontinuous. The best way to attack this problem would be to use a robust non-linear optimization technique that can handle the non-linearities associated with the simultaneous variation of pertinent material properties and can solve for the optimized compositional distribution which satisfies desired criteria. Numerous constrained optimization techniques are available that have been used in a variety of applications.

Another promising approach is based on applying neural networks developed for solving such optimization problems, i.e. the recurrent or feedback networks. Several forms of such networks exist that could be considered for application to FGM design. All are based on the following approach. First, the optimization criteria are expressed as functions that can be considered as cost or penalty functions. If these functions are written as an expression of the "energy" in the FGM system, and the various relationships can be expressed as a multidimensional field equation, then the optimum solution is the one that can be shown to be the minimum-energy solution. The most common of these networks is the Hopfield network that was formulated in terms of energy principles; thus extending the use of the neural network to a wider variety of applications. This is a fairly new approach to non-linear optimization, but one that appears to be of significant promise for FGM design.

4. In addition to neural networks, other established non-linear optimization methods should also be systematically considered. The "best" method may vary from one application to another, and ultimately we want to be able to choose the method that is best-suited to a given problem.

5. As an addendum to Points 3 and 4 above, the newly developing field of fuzzy logic may be useful as a practical FGM design tool. Fuzzy logic is an extension of the more traditional Boolean logic because it allows for partial truth and partial falsehood. It is particularly useful for modelling very complex systems that are difficult, or even impossible, to define completely. Its application to FGM design, with the associated complex microstructures and thermophysical-property models, therefore, appears to be a worthwhile approach. Indeed, a method of "fuzzy inference" was used by Tanaka *et al.* [25] in the calculation of thermophysical properties for an FGM.

6. In both modelling and experimental studies, what needs to be demonstrated is that the use of FGMs clearly results in superior performance relative to that obtained when "conventional", non-graded materials are used. Moreover, performance with FGMs must be evaluated against that achieved using the best available technology in conventional materials.

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