Numerical simulation of two-dimensional wave propagation in functionally graded materials

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Abstract

The propagation of stress waves in functionally graded materials (FGMs) is studied numerically by means of the composite wave-propagation algorithm. Two distinct models of FGMs are considered: i) a multilayered metal-ceramic composite with averaged properties within layers; ii) randomly embedded ceramic particles in a metal matrix with prescribed volume fraction. The numerical simulation demonstrates the applicability of that algorithm to the modelling of FGMs without any averaging procedure. The analysis based on simulation shows significant differences in the stress wave characteristics for the distinct models that can be used for optimizing the response of such structures to impact loading.

Key words: functionally graded material, wave propagation, numerical simulation, impulsive loading

1 Introduction

Functionally graded materials (FGMs) are widely used in contemporary technology because of their multifunctional properties. Analytical and computational studies of the evolution of stresses and displacements in FGMs subjected to quasistatic loading (Suresh et al., 1997; Suresh and Mortensen, 1998; Suresh, 2001; Pender et al., 2001) show that the utilization and optimization of structures and geometry of a graded interface between two dissimilar layers can reduce stresses significantly. Such an effect is certainly also important in case

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of dynamical loading where energy-absorbing applications are of special interest. One-dimensional stress wave propagation in FGMs is discussed by Liu, Han, and Lam (1999); Chiu and Erdogan (1999); Bruck (2000). The impact response of graded metal-ceramic plates in two dimensions is examined by Li, Ramesh, and Chin (2001). The response of FGM plates excited by impact loads in three dimensions is studied numerically by Han, Liu and Lam (2001). In these studies, FGMs are approximated by multilayered media, and material properties for each layer are assumed to be constant or to be expressed by linear or quadratic functions within a layer. One of the main difficulties in such an approach is the accurate estimation of material properties depending on the functionally varying volume composition of constituent particles. However, the FGMs are characterized not only by the presence and appearance of compositional or other gradients but also by the sophisticated behaviour of the FGM components in comparison with conventional (macroscopically uniform) materials. In the simplest case, the structure of a FGM can be represented by the model-like system of a matrix with embedded particles or grains.

In this paper, we focus on the analysis of the 2D stress wave propagation in the layered and graded metal-ceramic structures. As examples, structures are used which were examined by Li, Ramesh, and Chin (2001) with special reference to armour applications. We are interested, however, rather on the possible descriptions of FGMs than on the optimization of the structures. Therefore, we are restricted to only elastic wave propagation without any viscoplastic effects.

In what follows, computations are performed for two distinct models of FGMs:

- a multilayered metal-ceramic composite with averaged properties within layers;
- randomly embedded ceramic particles in a metal matrix with prescribed volume fraction.

The main aim of the paper is to compare the time evolution of the field quantities as a result of wave propagation and interaction with interfaces and gradients in these two models and clarify the significance of the choice of gradation on impact applications. It should be noted that different regimes of wave behaviour may be developed in structures with different physical size scales. We focus our attention on the case of dynamic loading of a plate where the wavelength of stress pulse is comparable with the plate thickness. This means that the wavelength is much larger than the size of inclusions and the distance of wave travel is relatively small. In addition, the rise time of the applied stress pulse is much larger than the ratio of the reinforcement dimension to the fastest wavespeed in the reinforcing material.
2 Formulation of the problem

A two-dimensional problem of the impulsive loading of a plate of thickness $h$ and length $L \gg h$ is considered. The load is applied transversally at the central region of the plate upper surface of length $a$ ($a < h$). The material of the plate is assumed to be compositionally graded along the thickness direction. The gradation is described in terms of the volume fraction of a ceramic reinforcing phase within a metal matrix. Following Li, Ramesh, and Chin (2001), three timescales of the problem can be introduced:

$$t_0 = \frac{h}{c_f}, \quad t_b = \frac{L}{c_f}, \quad t_r,$$

where $c_f$ is the speed of the fastest longitudinal wave, and $t_r$ is the shortest rise time, corresponding to the applied loading. Since $L \gg h$, it follows that $t_0 \ll t_b$, so that the lateral boundaries of the plate are not actually involved in the calculations. As pointed out by Li, Ramesh, and Chin (2001), if a volume fraction parameter alone is to be used to describe the gradation, then one must have $t_r \gg d_r/c_f$, where $d_r$ is the reinforcement dimension.

3 Governing equations for inhomogeneous elastic materials

Both metal and ceramics are assumed to behave as linear isotropic elastic media. In such a case, the governing equations of the problem can be represented in terms of stresses and velocities (Berezovski, Engelbrecht, and Maugin, 2000; Berezovski and Maugin, 2001) in a rather simple way:

$$\rho_0(x) \frac{\partial v_i}{\partial t} = \frac{\partial \sigma_{ij}}{\partial x_j},$$

$$\frac{\partial \sigma_{ij}}{\partial t} = \lambda(x) \frac{\partial v_k}{\partial x_k} \delta_{ij} + \mu(x) \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right),$$

Fig. 1. The geometry of the problem.
where $t$ is time, $x_j$ are spatial coordinates, $v_i$ are components of the velocity vector, $\sigma_{ij}$ is the Cauchy stress tensor, $\rho$ is the density, $\lambda$ and $\mu$ are the Lamé coefficients, $\delta_{ij}$ is the Kronecker delta. The indicated explicit dependence on the point $\mathbf{x}$ means that the body is materially inhomogeneous in general, i.e. the properties of graded materials are reflected in $\rho(\mathbf{x})$, $\lambda(\mathbf{x})$, and $\mu(\mathbf{x})$.

System of equations (2), (3) is a system of hyperbolic conservation laws in a form that is suitable for numerical simulations. We will solve this system of equations numerically with distributions of material properties corresponding to the multilayered model of metal-ceramic composite with averaged properties within layers and to the model of randomly embedded ceramic particles in a metal matrix with a prescribed volume fraction.

Assuming that the plate is at rest for $t \leq 0$, system of equations (2), (3) must be solved under the following initial conditions:

$$u_i(\mathbf{x}, 0) = 0, \quad \sigma_{ij}(\mathbf{x}, 0) = 0. \tag{4}$$

The upper surface of the plate is subjected to a stress pulse given by

$$\sigma_{22}(x, 0, t) = \sigma_0 \sin^2(\pi(t - 2t_r)/2t_r), \quad -a/2 < x < a/2, \quad 0 < t < 2t_r. \tag{5}$$

Other parts of upper and bottom surfaces are stress-free, lateral boundaries are assumed to be fixed.

4 Material properties

In order to compute the overall strain/stress distributions in FGMs, one needs the appropriate estimates for properties of the graded layer, such as the Young’s modulus, Poisson’s ratio, etc. A large number of papers on the prediction of material properties of FGMs has been published (see, for example, Gasik (1998); Cho and Oden (2000); Cho and Ha (2001)). In most of these studies the averaging methods have been used which are simple and convenient to predict the overall thermomechanical response and properties, however, owing to the assumed simplifications, the validity of simplified models in real FGMs is affected by the corresponding detailed microstructure and other conditions. Still, the averaging methods may be selectively applied to FGMs subjected to both uniform and non-uniform overall loads with a reasonable degree of confidence.

As was pointed out in introduction, our main goal is to compare two distinct models of FGMs: (i) a multilayered model of a metal-ceramic composite with
averaged properties within each layer and (ii) a model of the same composite with randomly embedded ceramic particles in a metal matrix. For this purpose, it is sufficient to employ the linear rule of mixtures for the Young’s modulus and Poisson’s ratio of the graded layer in the multilayered model of metal-ceramic composite with averaged properties within layers. According to the linear rule of mixtures, the simplest estimate of any material property, a property \( P(\mathbf{x}) \) at a point \( \mathbf{x} \) in dual-phase metal-ceramic materials is approximated by a linear combination of volume fractions \( V_m \) and \( V_c \) and individual material properties of metal and ceramic constituents \( P_m \) and \( P_c \):

\[
P(\mathbf{x}) = P_m V_m(\mathbf{x}) + P_c V_c(\mathbf{x}).
\]  

The same individual material properties without any averaging are used in the model of the composite with randomly embedded ceramic particles in a metal matrix.

## 5 Numerical algorithm

It should be noted that there exist many algorithms used for the numerical solution of hyperbolic systems of equations. But, certain assumptions about the smoothness of solutions are typically used in order to approximate derivatives in standard finite-difference methods. These approximations, however, are not valid near discontinuities in the material parameters. Therefore, standard methods often fail completely if the parameters vary drastically on the grid size. By contrast, the recently developed wave-propagation algorithm (LeVeque, 1997) has been found quite natural for the modelling of wave propagation in rapidly-varying heterogeneous media (Fogarty and LeVeque, 1999). This algorithm combines the high-resolution with multi-dimensionality of wave propagation. Special limiter functions are applied to reduce spurious oscillations near discontinuities. As a result, the sharp resolution of shocks along with nearly second-order accuracy of smooth solutions is obtained (LeVeque, 1997).

An improved composite wave propagation scheme where a Godunov step is performed after several second-order Lax-Wendroff steps was successfully applied for the two-dimensional thermoelastic wave propagation in media with rapidly-varying properties (Berezovski, Engelbrecht, and Maugin, 2000; Berezovski and Maugin, 2001). This scheme is also applied here. We believe that this scheme is a powerful tool for studying the various FGMs.
6 Computational results

6.1 One-dimensional case

First we consider the stress wave propagation in the one dimensional setting. This simplification is motivated to draw the parallels with a similar problem discussed by Cermelli and Pastrone (2000) who have shown the possible decay of the wave amplitude by a layer where some microscopic damage has been accumulated. Their model was based on the concept of internal variables (cf. also Engelbrecht, Cermelli, and Pastrone (1999)). Microstructure is then described by a certain scalar field that depends on the defect density and affects the energy function. It results in a certain additional nonequilibrium stress accounted for in governing equations (Cermelli and Pastrone, 2000).

![Graph](image)

Fig. 2. Stress wave propagation inside a medium with inhomogeneous layer (multi-layered model with averaged properties within layers): a) change in the properties of the material, b) stress profiles for consecutive time instants (150 time steps delay between profiles).

In our calculation, a FGM layer is placed in the interval [300,700] within the dimensionless computational domain [0,1000] - see Fig. 2a, 3a. The mechanical properties of the layer are either (i) smoothly changing from the ceramic (Al$_2$O$_3$) to metal (Ni) (Fig. 2a) and the change taken in the form of the Gaus-
sian distribution or (ii) given by a mixture of randomly embedded particles with the same Gaussian distribution function (Fig. 3a). The properties of the metal and ceramic are the following (Cho and Oden, 2000; Cho and Ha, 2001): Young’s modulus 199.5 GPa and 393 GPa, Poisson’s ratio 0.3 and 0.25, and density 8900 kg/m³ and 3970 kg/m³, respectively.

Fig. 3. Stress wave propagation inside a medium with inhomogeneous layer (model with randomly embedded particles): a) change in the properties of the material, b) stress profiles for consecutive time instants (150 time steps delay between profiles).

The results of calculations are shown in Figs. 2b, 3b. Clearly we get an expected decreasing of the transmitted wave amplitude after interaction with the layer. It should be noted that the remarkable decreasing is observed only in the case of significant difference in the properties of materials. This effect manifests itself more clearly if we model the inhomogeneous layer by randomly embedded particles (Fig. 3b). In addition, due to the random distribution in the layer, the reflected wave shows up certain irregularities (small wiggles about the zero line) that can be used for detecting the properties of the layer. By comparing the results obtained by the formalism of internal variables (Cermelli and Pastrone, 2000) and straightforward calculations, one could determine the properties of the scalar field used to model internal variables.
Fig. 4. Density distribution in metal-ceramic composite with ceramic reinforcement corresponding to the multilayered model with averaged properties within layers: a) uniform, b) layered, c) continuously graded (high $f$ front), d) continuously graded (low $f$ front) (after Li, Ramesh, and Chin (2001)).

6.2 Two-dimensional case

Now we return to the 2-D plane strain problem formulated in Sect. 2. We consider four possible forms of the ceramic particulate reinforcement volume fraction variation along the thickness in the case of the multilayered model with averaged properties within layers: uniform, layered, and graded with two different distributions of volume fraction $f = V_c$ (Fig. 4), where the elastic properties of the metal matrix and ceramic reinforcement are the following (Li, Ramesh, and Chin, 2001): Young’s modulus 70 GPa and 420 GPa, Poisson’s ratio 0.3 and 0.17, and density 2800 kg/m$^3$ and 3100 kg/m$^3$, respectively. These structures are examined as the Cases A, B, C and D by Li, Ramesh, and Chin (2001) in the axisymmetric case. Simultaneously, the same structures are represented by randomly embedded ceramic particles with the corresponding volume fraction (Fig. 5).

The same algorithm was applied for the numerical simulation of stress wave propagation in both models. In computation, we used 98 elements in the thickness direction, so that the reinforcement dimension was as long as 250 $\mu$m. The rise time $t_r$ for the loading was chosen as 0.75 $\mu$s. This satisfies the condition $t_r \gg d_r/c_f$, because the speed of the fastest longitudinal wave is equal to 11877 m/s corresponding to the data by Li, Ramesh, and Chin (2001). Typical examples of contour plots showing the full displacement fields are presented in Fig. 6. Computations performed under the same conditions for distinct models
Fig. 5. Random particle distribution in metal-ceramic composite with ceramic reinforcement: e) uniform, f) layered, g) graded (high $f$ front), h) graded (low $f$ front).

of the same FGM: $L = 49 \, mm$, $h = 24.5 \, mm$, $a = 12.25 \, mm$, $\sigma_0 = 125 \, MPa$.

The difference in the propagation speed of stress wave is clearly seen whereas the particle volume fraction was distributed similarly in both models. In addition, we have the distortion of the symmetrical shape of the wavefronts in the model with randomly embedded particles due to random particle distribution.

One of the issues of interest in the use of layered or graded structures, for example, for armour applications was formulated by Li, Ramesh, and Chin (2001) as follows: What is the effect of the layering or gradation on maxima of stresses and their distributions? This is important in order to optimize the structure relative to integrity under dynamic loading. In attempt to answer the formulated question, let us consider the normal stress distribution along the centerline of the plate where maximal values of stress are expected.

6.2.1 Centerline stress distribution

The normal stress distribution along the centerline for the multilayered model with averaged properties within layers is shown in Fig. 7. Since the results are given at the same instant of time, the difference in the position of normal stress profiles characterizes the corresponding difference in the speed of the stress wave in each structure in the full accordance to the mean volume fraction of ceramic particles in each structure (0.360 for the uniform distribution, 0.226 for the layered case, 0.475 for the high $f$ front, and 0.120 for the low $f$
Fig. 6. Wavefronts in metal-ceramic composite with ceramic reinforcement at 3 μs: a) multilayered model with averaged properties within layers (case c, Fig. 4), b) model with randomly embedded ceramic particles (case g, Fig. 5).

Obviously the alternating layering (case b) results in the decrease of the amplitude and of the transmitted wave compared with the homogenized case (a). The maximal tensile stresses are considerably higher for the layered case. Continuous grading yields the following (see Fig. 7). There is no significant differences in maximal amplitudes between the high and low front grading (cases c, d) but there is a large difference in speeds. This effect is due to the material properties of the corresponding ceramic reinforcement.

The huge tensile stresses in the layered material due to the reflection through the structure dictates its rejection in order to provide the improvement of the integrity of the structure under dynamic loading. The situation is slightly changed for the model of randomly embedded particles (Fig. 8). Here the
Fig. 7. Normal stress distribution along the centerline in metal-ceramic composite with ceramic reinforcement at 3 μs (multilayered model with averaged properties within layers).

Fig. 8. Normal stress distribution along the centerline in metal-ceramic composite with ceramic reinforcement at 3 μs (model with randomly embedded particles).

difference in the speed of propagation of the stress waves in distinct structures is much less but the difference in their amplitudes became higher. Due to the high percentage of ceramic reinforcement in case c), the speed of the longitudinal wave keeps the highest value in all the calculated cases. The amplitude of the tensile stresses decreases significantly, especially for uniform and low f front grading (cases e) and h)). It seems that the latter structure (case h)) is the best choice for the damping both the compressional and tensile stresses. This result is not so obvious in the case of the multilayered model with averaged properties within layers.
Theoretical prediction of dynamic behaviour of FGMs depends on how well their properties are modelled in computer simulations. While many averaging models of the properties of FGMs are widely accepted, a more natural model of a matrix with randomly embedded particles was never used because of numerical difficulties in the case of rapidly-varying properties of the medium. This difficulty is overcome by using the wave-propagation algorithm (LeVeque, 1997) and its modifications (Berezovski, Engelbrecht, and Maugin, 2000; Berezovski and Maugin, 2001). Within the composite wave-propagation algorithm, every discontinuity in parameters is taken into account by solving the Riemann problem at each interface between discrete elements. The reflection and transmission of waves at each interface are handled automatically for the considered inhomogeneous media.

In this paper, we applied the composite wave-propagation algorithm (Berezovski, Engelbrecht, and Maugin, 2000; Berezovski and Maugin, 2001) to compare the models of discrete layers with averaging the material properties and of randomly embedded ceramic particles in a metal matrix. The results of performed numerical simulations of stress wave propagation in FGMs show a significant difference between characteristics of wave fields in the distinct models, though the overall wavefronts picture (Fig. 6) seems similar in both cases. This means that a model of FGM without averaging of material properties can give a more detailed information about the dynamic behaviour of a chosen structure, which may be used in its optimization for a particular situation.

It should be noted that the size, the shape, the clustering, and inhomogeneities in the random distribution of embedded reinforcement particles may affect the results of simulation in each particular case. Nevertheless, at least some of the mentioned effects can be easily taken into account by means of the developed numerical scheme. Further studies are in progress.

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Figure captions

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Fig 6. Wavefronts in metal-ceramic composite with ceramic reinforcement at 3 $\mu$s: a) multilayered model with averaged properties within layers (case c), Fig. 4), b) model with randomly embedded ceramic particles (case g), Fig. 5).

Fig 7. Normal stress distribution along the centerline in metal-ceramic composite with ceramic reinforcement at 3 $\mu$s (multilayered model with averaged properties within layers).

Fig 8. Normal stress distribution along the centerline in metal-ceramic composite with ceramic reinforcement at 3 $\mu$s (model with randomly embedded particles).
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