10-28-2008

Design of Functionally Graded Materials Using Transient Nonlinear Simulations and Genetic Algorithm Optimization

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Final Report for Period: 08/2007 - 07/2008
Submitted on: 10/28/2008
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Award ID: 0423485
Organization: University of Maine
Submitted By:
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Title:
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Project Participants

Senior Personnel

Name: Vel, Senthil
Worked for more than 160 Hours: Yes
Contribution to Project:

Post-doc

Graduate Student

Name: Goupee, Andrew
Worked for more than 160 Hours: Yes
Contribution to Project:

Name: Pelletier, Jacob
Worked for more than 160 Hours: Yes
Contribution to Project:

Name: Baskiyar, Rajeev
Worked for more than 160 Hours: Yes
Contribution to Project:

Undergraduate Student

Technician, Programmer

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Research Experience for Undergraduates

Organizational Partners

Other Collaborators or Contacts

Activities and Findings

Research and Education Activities:

Functionally graded materials (FGMs) are macroscopically inhomogeneous multicomponent material systems that are engineered to have a smooth spatial variation of material properties. This is achieved by gradually varying the microstructure and relative volume fractions of the constituent material phases from one point to another. FGMs are typically lighter and stronger than monolithic components. The goal of this research is to develop a robust methodology for tailoring the spatial material composition and microstructure of functionally graded materials for high temperature and high heat flux applications by synergistically combining material constituents, performing accurate numerical simulations to evaluate candidate designs and mathematical optimization. The research activities have focused on,

1) Multiscale Analysis of Functionally Graded Materials:
In order to design superior functionally graded materials, it is important to compute their effective material properties and strength accurately. Although there has been significant amount of research to date on functionally graded materials, most of the analyses use rudimentary schemes to evaluate their effective properties. Some of the widely used homogenization schemes, including the rule-of-mixtures, the Mori-Tanaka method and the self-consistent scheme, are not very accurate since they are based solely on the relative volume fractions of the constituent phases and they do not account for the material microstructure (i.e. material arrangement at the microscopic level).

We have developed a multiscale methodology for the accurate analysis of functionally graded materials based on a two-scale asymptotic homogenization technique. The material is assumed to have a locally periodic microstructure although it can be macroscopically inhomogeneous with different microstructures at different locations. The temperature and stresses are assumed to be functions of both the macroscale and the microscale coordinates. The microscale problem is analyzed by the finite element method using a mesh that conforms to the irregular shape of the interface between the material constituents. The effective thermal conductivity, thermal expansion coefficient and elastic moduli obtained by the multiscale technique are used to assess the accuracy of simple homogenization schemes for various microstructures.

2) Analysis of Functionally Graded Materials with Random Microstructure:
Micrographs of functionally graded materials exhibit significant randomness and complex microstructures. However, most homogenization theories for functionally graded materials assume a simple microstructure to obtain the effective material properties. For example, the Mori-Tanaka effective medium theory assumes that the microstructure consists of spherical or elliptical inclusions embedded in a matrix. In order to design functionally graded components, it is important to develop accurate models for the homogenized material properties and strength of random media. However, there has been a lack of research on functionally graded materials with random microstructure. We have developed a computational technique to generate random microstructures with complex morphology. The microstructure of the random multicomponent materials is described using newly developed morphology description functions. The interface between the material phases is obtained by performing a level cut through the morphology description function at a threshold value. A location within the microstructure is assigned a specific material phase depending on whether the value of the morphology description function is less than or greater than the threshold value. Different microstructures and phase volume fractions can be obtained by varying the threshold value. The homogenized material properties and failure envelopes for different volume fractions of the constituent material phases are computed using the multiscale analysis technique developed earlier.

3) Transient Multiscale Simulation and Optimization of Functionally Graded Materials:
Optimization of functionally graded materials typically involves the evaluation of thousands of candidate designs. It is therefore critical to develop a simulation tool for the rapid analysis of functional graded materials. We have developed an efficient code for the transient multiscale analysis of functionally graded materials under prescribed thermomechanical loads and boundary conditions. The macroscopic transient thermoelastic response of the functionally graded material is simulated using the element-free Galerkin method. Here, the material properties at the each quadrature point are evaluated using multi-scale analysis. The macroscopic stresses are then transferred to the microscale to obtain the microscopic stresses. Subsequently, the factor of safety is computed at the microscopic level using appropriate failure theories for the individual material phases. The microstructure and material distribution of functionally graded components are simultaneously optimized using an elitist, non-dominated sorting multi-objective genetic algorithm.

4) Optimization of Material Composition:
We have developed a multi-objective optimization algorithm for the optimization of material composition of bi-directional FGMs. The material distribution over the domain is described using the volume fraction of one of the constituent phases at a finite number of control points. The volume fraction values at other locations are obtained by range restricted interpolation. The effective material properties are obtained from the local volume fractions of the constituent phases through homogenization using rigorous micromechanical models. The temperature dependence of the thermal and thermomechanical material properties are taken into account and the two-dimensional heat conduction and thermoelasticity problems are solved using the element-free Galerkin method. The volume fractions at the control points are optimized using a non-dominated sorting genetic algorithm. The genetic algorithm has the ability to handle complex constraints and obtain globally optimal designs. It shows good convergence and it yields a well distributed set of designs on the Pareto-optimal frontier.

5) Analysis and Design of Orthotropic Functionally Graded Shells and Tubes:

We are also interested in the design of functionally graded shells and tubes for high temperature applications. In order to analyze isotropic and fiber-reinforced functionally graded thick shells and tubes, we have developed a three-dimensional solution to the heat conduction and thermoelasticity equations for cylindrical geometries. The material composition and fiber orientations can be arbitrary functions of the radial coordinate of the shell. The material properties are expanded as Taylor series in the radial direction and the temperature, heat flux, displacements and thermal stresses are obtained using a power series solution. A multi-objective optimization algorithm is used to optimize the radial distribution of material properties in order to maximize the strength of the tube while simultaneously minimizing its weight.

Findings:

We have developed a program for the simulation based design of functionally graded materials. The results demonstrate that the proposed methodology, which utilizes a multiscale analysis technique, is robust and it can be used to design functionally graded components with superior thermomechanical properties. We have found that,

1) The temperature, heat flux and stresses in a functionally graded material can be computed accurately using multiscale analysis since it links the micro- and macro-scales phenomena. The technique, which takes into consideration the arrangement of material phases at the microscale, provides reliable estimates for the homogenized material properties. Furthermore, the temperature and stresses can be determined within the individual constituent materials of the functionally graded material. The microscopic stresses, when used in conjunction with appropriate failure theories for the constituent phases, are useful in analyzing the strength of the material. The effective thermal conductivity, thermal expansion coefficient and Young's modulus obtained by the multiscale technique are used to assess the accuracy of some of the widely used homogenization theories. It is found that the Mori-Tanaka scheme is more accurate than other homogenization theories for multi-component microstructures with well-defined matrix and particulate phases. However, the Mori-Tanaka scheme provides inaccurate results for interpenetrating/skeletal microstructures.

2) Random microstructures that are generated using morphology description functions compare favorably with micrographs for the entire range of volume fractions. They are able to reproduce the interpenetrating microstructures when the volume fractions of the constituent phase are nearly equal. The synthetic random microstructures are statistically isotropic with a characteristic length scale that decreases with an increase in the number of Gaussian sources used in the morphology description functions. The synthetic microstructures percolate at a volume fraction of 1/2. The microscopic stress fields exhibit significant stress concentrations as expected. Thousands of random microstructures were generated and analyzed to obtain representative failure envelopes for the efficient analysis and design of functionally graded materials.

3) The results demonstrate that the proposed multi-objective optimization algorithm can handle arbitrary objective functions and non-linear constraints to yield a set of Pareto-optimal designs. We have applied the methodology to design the material composition of Zirconia/Titanium FGMs subjected to high temperatures and Tungsten/Copper FGMs under extremely high heat fluxes. The optimized FGMs exhibit higher factors of safety, lower weight and lower temperatures than obvious linearly graded FGMs. The results indicate that it is important to take into account the temperature dependence of the material properties. Due to the large variation in temperatures from one point on the body to another, the material properties also exhibit a substantial spatial variation. This is turn has a considerable affect on the thermal stresses. In addition, the temperature has a significant effect on the yield strength of the metal due to thermal softening. Thus, in order to accurately compute the factor of safety of candidate designs, the temperature dependence of the material properties must be taken into account.

4) Analytical solutions for the analysis of FGM shells and tubes that are graded in the radial direction are found to be very accurate and they are useful for the rapid evaluation of candidate designs. The effectiveness of the analysis and optimization methodology is demonstrated using two model problems. In the first model problem, functionally graded Zirconia/Titanium plates and shells are subjected to a sinusoidal temperature load on the top surface. They are optimized for minimum hoop stress and minimum mass subject to a constraint on the maximum temperature experienced by the Titanium phase. It is found that significant reductions in hoop stress are obtainable, while only moderately increasing the mass of the plate or shell. In the second model problem, a set of Pareto-optimal designs is obtained for Tungsten/Copper isotropic plates and shells subjected to sinusoidal heat flux on the top surface, while the remaining surfaces were maintained at the reference temperature. A range of volume fraction profiles are obtained that offer varying degrees of strength and mass.

Training and Development:

One Ph.D. student and one M.S. student had the opportunity to work on this project during the last year:

* Mr. Andrew J. Goupee worked on the analysis and genetic algorithm optimization of isotropic functionally graded materials. He defended his M.S. thesis in August 2005 and he is currently a doctoral candidate in our program. He has made good progress on the multiscale analysis and optimization of functionally graded materials. He has published 3 journal papers and 2 conference papers to date. He is in the process of writing up his work on random functionally graded materials for publication in a refereed journal.

* Mr. Jacob L. Pelletier worked on the analysis and optimization of fiber-reinforced functionally graded shells. He defended his M.S. thesis in August 2005. He has published 2 journal papers based on his thesis and 1 more journal paper is currently in review.

* Mr. Rajeev Baskiyar worked on the analysis and design of fiber-reinforced functionally graded anisotropic tubes. The goal of his research was to design FGM tubes that can withstand thermal shock. He has published one conference paper.

Outreach Activities:

Nothing to Report

Journal Publications

Andrew J. Goupee and Senthil S. Vel, "Two-dimensional Optimization of Material Composition of Functionally Graded Materials using Meshless Analyses and a Genetic Algorithm", Computer Methods in Applied Mechanics and Engineering, p. 5926, vol. 195, (2006). Published,

Jacob L. Pelletier and Senthil S. Vel, "An Exact Solution for the Steady-State Thermoelastic Response of Functionally Graded Orthotropic Cylindrical Shells", International Journal of Solids and Structures, p. 1131, vol. 43, (2006). Published,

Andrew J. Goupee and Senthil S. Vel, "Optimization of Natural Frequencies of Bidirectional Functionally Graded Structures", Structural and Multidisciplinary Optimization, p. 473, vol. 32, (2006). Published,

Andrew J. Goupee and Senthil S. Vel, "Multi-objective Optimization of Functionally Graded Materials with Temperature-dependent Material Properties", Materials & Design, p. 1861, vol. 28, (2007). Published,

Senthil S. Vel and Jacob L. Pelletier, "Multi-objective Optimization of Functionally Graded Thick Shells for Thermal Loading", Composite Structures, p. 386, vol. 81, (2007). Published,

Jacob L. Pelletier and Senthil S. Vel, "Multi-objective Optimization of Fiber Reinforced Composite Laminates for Strength, Stiffness and Minimal Mass", Computers & Structures, p. 2065, vol. 84, (2007). Published,

Books or Other One-time Publications

Senthil S. Vel and Andrew J. Goupee, "A Methodology for the Optimization of Material Composition of Functionally Graded Materials", (2005). Conference article, Published
Bibliography: Proceedings of the NSF Design, Service and Manufacturing Grantees and Research Conference, Scottsdale, Arizona, Jan 3-6, 2005

Senthil S. Vel and Andrew J. Goupee, "Multi-objective optimization of geometric dimensions and material composition of functionally graded components", (2008). Conference article, Published
Editor(s): G. H. Paulino, M.-J. Pindera, R. H. Dodds, Jr., F. A. Rochinha, E. V. Dave, and L. Chen
Bibliography: Proceedings of the Multiscale and Functionally Graded Materials Conference 2006, Honolulu, Hawaii. American Institute of Physics, 978, pp. 610-615, 2008.

Senthil S. Vel and Rajeev Baskiyar, "Thermally induced stresses in functionally graded thick tubes", (2008). Conference article, Published
Editor(s): G. H. Paulino, M.-J. Pindera, R. H. Dodds, Jr., F. A. Rochinha, E. V. Dave, and L. Chen
Bibliography: Proceedings of the Multiscale and Functionally Graded Materials Conference 2006, Honolulu, Hawaii. American Institute of Physics, 978, pp. 688-693, 2008.

Senthil S. Vel and Andrew J. Goupee, "A Methodology for the Optimization of Material Composition of Functionally Graded Materials", (2005). Conference article, Published
Bibliography: Proceedings of the 2005 NSF Design, Service and Manufacturing Grantees and Research Conference, Scottsdale, Arizona.

Senthil S. Vel, Andrew J. Goupee, Jacob L. Pelletier, "Multi-objective Design Optimization of Functionally Graded Materials", (2006). Conference article, Published
Bibliography: Proceedings of the 2006 NSF Design, Service, and Manufacturing Grantees and Research Conference, St. Louis, Missouri

Senthil S. Vel and Andrew J. Goupee, "Multiscale Design of Functionally Graded Materials", (2008). Conference article, Published
Bibliography: Proceedings of the 2008 NSF CMMI Engineering Research and Innovation Conference, Knoxville, Tennessee

Jacob L. Pelletier, "Thermoelastic Analysis and Optimization of Functionally Graded Plates and Shells", (2005). Thesis, Published
Bibliography: M.S. Thesis, University of Maine

Andrew J. Goupee, "Methodology for the Thermomechanical Simulation and Optimization of Functionally Graded Shells", (2005). Thesis, Published
Bibliography: M.S. Thesis, University of Maine

Web/Internet Site

URL(s):
http://www.umaine.edu/mecheng/vel/research/FGM_design.htm
Description:

Other Specific Products

Contributions

Contributions within Discipline:

We have made fundamental contributions to the mechanics and design of functionally graded materials.

1) Mechanics of functionally graded materials:
The multiscale technique provides a fundamental understanding of the response of functionally graded materials. We have proposed novel morphology description functions to generate realistic random microstructures. Homogenized material properties and failure envelopes have been generated for representative functionally graded materials with random microstructure. In addition, an efficient multiscale technique has been developed for the accurate transient analysis of functionally graded materials.

2) Design of functionally graded materials:
We have developed an integrated methodology for the optimization of FGMs based on accurate numerical simulations and a global optimization technique using genetic algorithms. Such a unified framework will enable engineers and other professionals engaged in the design process with FGMs to develop superior mechanical components by synergistically combining menus of material ingredients, fabrication processes, three-dimensional transient numerical simulations and optimized material distribution.

Contributions to Other Disciplines:

Nothing to report

Contributions to Human Resource Development:

Work by three graduate students involved in this project has led to the development and advancement of their knowledge on issues related to the analysis of mechanical components with complex material distributions. The analysis and multi-objective optimization skills that they have developed through this project will prove to be useful when designing a variety of engineering systems.

Contributions to Resources for Research and Education:

Nothing to report

Contributions Beyond Science and Engineering:

Nothing to report

Conference Proceedings

Categories for which nothing is reported:

Organizational Partners

Any Product

Any Conference