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13. ABSTRACT (Maximum 200 words)

After three years of the project, many of the proposed research topics have been completed and manuscripts were submitted for publication. First, for the dynamic crack propagation within functionally graded materials (FGMs), a novel fracture criterion was introduced. It is based on energy concept and controls crack growth rate and associated plastic dissipation flow. This model was implemented in dynamic failure analysis to investigate crack propagation within elastic plastic graded materials. The new procedure was also implemented for the impact of graded protective layer. The results confirmed the importance of modeling of cracking, revealed the effects of compositional gradation through-thickness. In a subsequent analysis, a procedure that utilizes an inverse analysis was developed to measure key fracture parameters. These parameters are difficult to measure with conventional means. Third, in collaboration with materials science group, material parameters of actual FGM were measured using the indentation and inverse method. The specimens were thermal barrier coatings fabricated with zirconia and NiCrAlY. This type of advanced scheme to post-process experimental data is essential for obtaining properties of complex systems. In addition, preliminary fracture tests were conducted for thicker FGMs to determine its fracture behavior.

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Sincerely,

FINAL PROGRESS REPORT

Optimizing Functionally Graded Materials to Resist Failure under Dynamic Loadings

ARO funded project 1999 – 2002

Foreword

Various aspects of graded materials were investigated under the funding of the U.S. Army Research Office. These studies are the first of kind for *elastic-plastic* FGM's and the support of ARO is gratefully acknowledged.

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Project Objectives

The project's aims were to develop necessary computational tool to optimize functionally graded materials. In particular their failure characteristics were to be elucidated under dynamic conditions. Furthermore, new data processing techniques to determine key parameters necessary to define their failure conditions were established. Such techniques to integrate computational and experimental means are indispensable for complex materials where direct correlations with measured data to material parameters are often unachievable.

Summary of Results

Recent advances in materials processing techniques have enabled the cost-effective fabrication of inhomogeneous materials including those classified as functionally graded materials. Using advanced modeling approaches, the compositions and material properties of graded materials can be suitably tailored and designed to produce performance maximized for specific applications. For example, liners of gun barrels and lightweight ballistic resistant layers are potential military applications of FGM's. In the project, a new criterion for crack growth of graded materials was proposed. Due to the spatial variations of material properties, conventional fracture criteria cannot be directly applied to FGM's. This criterion assumes a certain relationship between the separation energy and the peak stresses needed to generate new surfaces. This was implemented in a finite element code and simulations were carried out to test its accuracy. This type of analysis is needed for the optimization of FGM performance. It enables the characterization of failure resistant behavior under dynamic loading and establishes a linkage between *micro-scale cracking/damage* and *large-scale fracture* of FGM with a smooth transition across the multi-scale stages of failure.

During this period of the research project, several accomplishments were made. First, the simulation work on dynamic FGM fracture, including formulation for property determination, was refined and completed (Nakamura and Wang, 2001, Wang and Nakamura, 2002). Manuscripts have been also prepared. Second, experimental investigation was carried out on real FGM with micro-indentation, and our new procedure based on inverse analysis was implemented (Nakamura and Sampath, 2000, 2001; Gu et al., 2002). The results confirmed the effectiveness of this technique. Third, fracture tests on thick FGM layer were conducted. Although it was an initial study, a toughening behavior was observed as crack propagated. These studies are summarized below. More details are discussed in the referenced papers.

One of major progresses made during this period was accurate formulation for dynamic crack propagation of FGM using physically consistent models. Simulations were carried out with double cantilever beam configuration (Fig. 1). The proposed criterion assumes the power law relationship between the separation energy G_o and the peak stress $s_{\max}$ required to generate new crack surfaces.

$$\frac{s_{\max}}{s^{*}_{\max}} = \left(\frac{G_o}{G_o^{*}}\right)^{a} . \tag{1}$$

Here G_o* and $s_{\max}$* are the parameters defined at a reference point (e.g., elastic phase). The exponent a can be any real number that defines the variation of $s_{\max}$ as a function of G_o. Without the above relation, independent measurements of spatial variant G_o and $s_{\max}$ would be extremely complex.

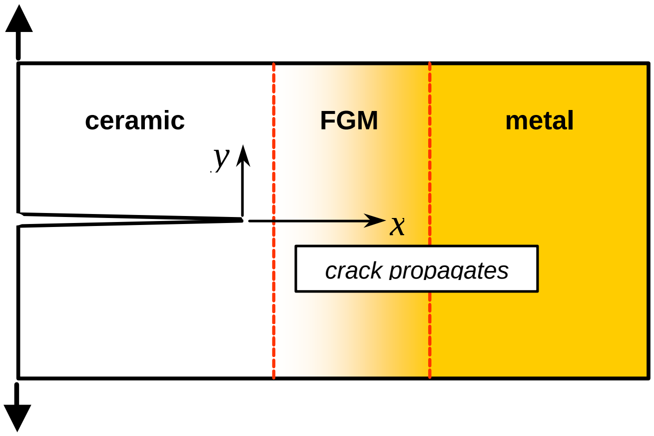

Fig. 1. Double cantilever beam model for dynamic FGM crack simulations.

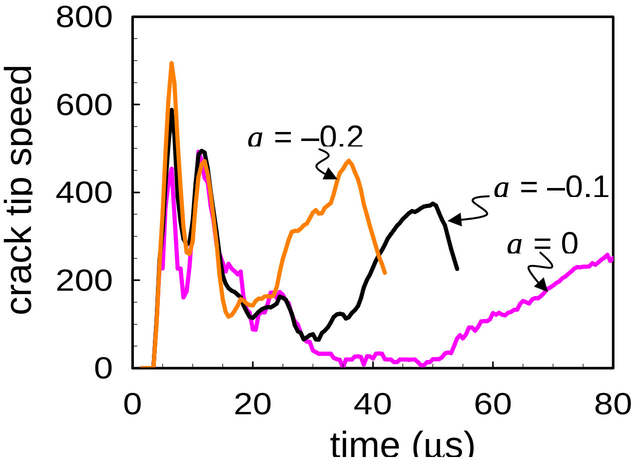

Fig. 2. Variations of crack speed for different criteria.

Computed results show highly dependent nature of crack propagation on the variation of $s_{\max}$ defined through the exponent a (Fig. 2).

Using the computational procedure established for the crack propagation in graded materials, a more complex dynamic failure behavior is analyzed. Here a FGM model under high velocity rod impact is considered. Unlike the previous model with well-defined crack path, the impact generates multiple crack nucleations at arbitrary locations and growths along arbitrary directions. The impact load model consisting of a protective FGM layer and a metal substrate (Fig. 3). This is a simplified model and not meant to simulate actual projectile striking or penetration phenomena of real armors. However, the model is sufficient to verify the explicabilities of the current failure procedure for graded materials in complex boundary value problems.

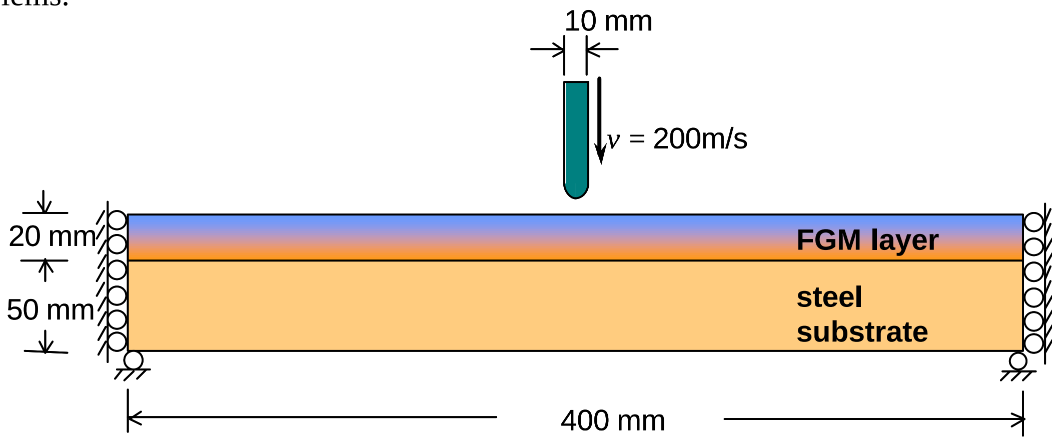

Fig. 3. Schematic of protective FGM layer and substrate subjected to impacting rod.

The impact generates high stresses that induce fracturing underneath the impact. The stress state at 8μs after the impact is shown in Fig. 4.

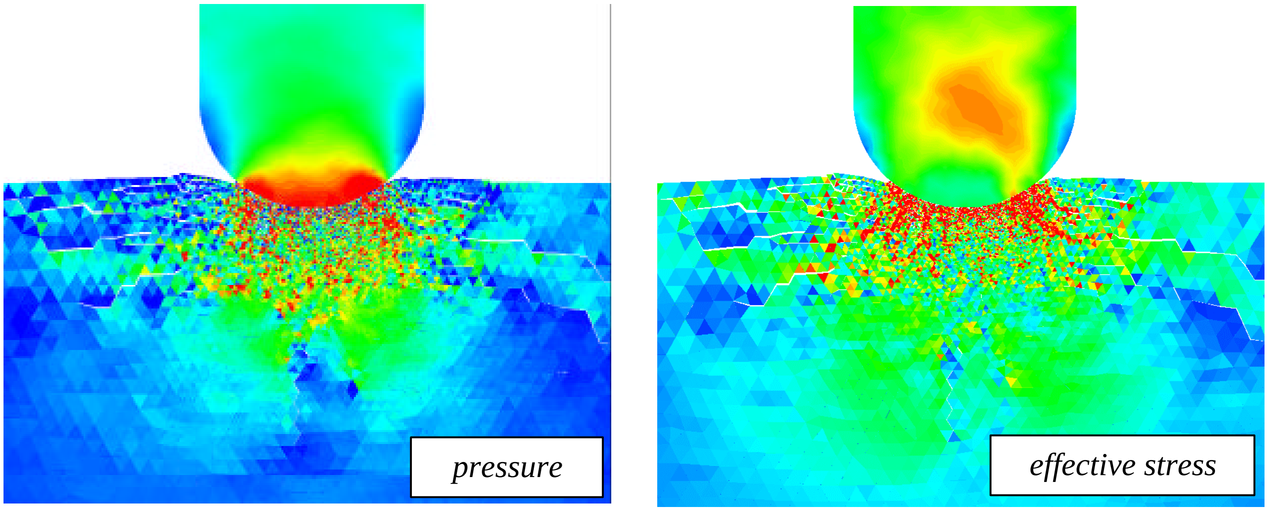

Fig. 4. Shades of stresses at t = 8μs after impact shown for pressure and effective stress Discontinuous stresses are due to cracking.

In order to quantify the effects of material gradation on fracture behaviors. The geometry, loading conditions and material properties of ceramic and metal are kept the same while different compositional gradations are prescribed. To describe the gradation conveniently, the variation of material composition is set to follow the power-law relation as,

$$V_{\mathrm{m}} = (z / d)^{n}. \tag{2}$$

Here, V_m is the volume fraction of metal phase, z is the distance measured from the top surface, d is the thickness of the FGM layer (d = 20mm), and n is the material gradation parameter. The metal volume fraction is always $V_m = 0$ at $z = 0$, and $V_m = 1$ at $z = d$. The crack profiles for n = 1/3 and 3 are shown in Fig. 5. The energy transfer from the external work (e.g., kinetic energy of rod) to various internal energy components including the dissipative energy (fracture energy plus plastic flow) are shown in Fig. 4.

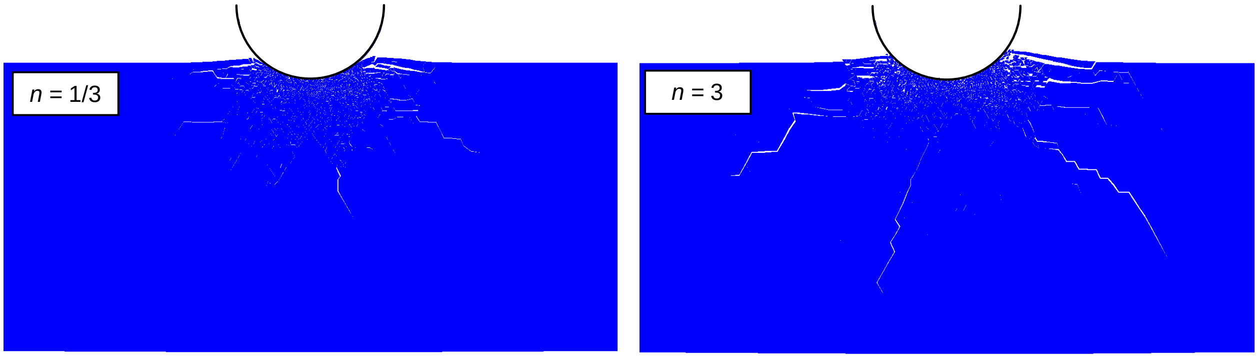

Fig. 5. Crack profiles at t = 8μs for n = 1/3 and 3 gradations. Greater vertical cracks are observed with larger n.

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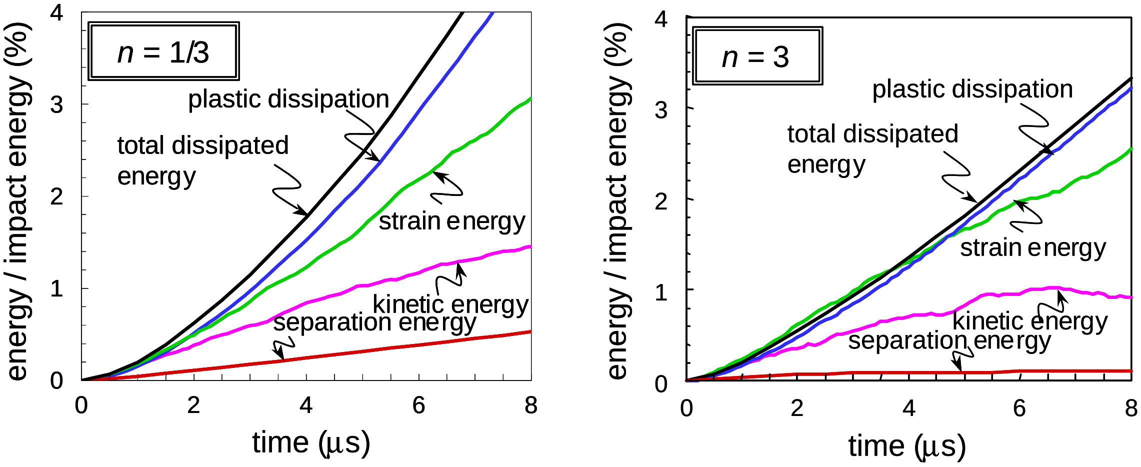

Fig. 6. Evolutions of various energy components in the FGM layer shown for various gradations for n = 1/3 and 3. Total dissipation is the sum of separation and plastic energies.

In addition, mode dependency on the fracture criterion was also investigated. With larger Mode II toughness, the initiations are delayed significantly and different energy evolutions are observed. In all cases, the energy directly consumed by crack formations represent a small part of overall energy. However, the presence of cracks significantly alters the other energy components, including the plastic dissipation. These results attest the importance of accurate crack modeling in similar boundary value problems.

Before actual FGM or functional materials can be utilized in real applications, their properties must be identified. However, due to the complexity of the material system, any procedures to quantify the properties can be very elaborated. In order to alleviate such difficulties, a new measurement procedure based on the inverse analysis was also introduced. This procedure uses the Kalman filter to make best estimates of fracture properties of FGMs. The flow chart of this procedure is shown in Appendix

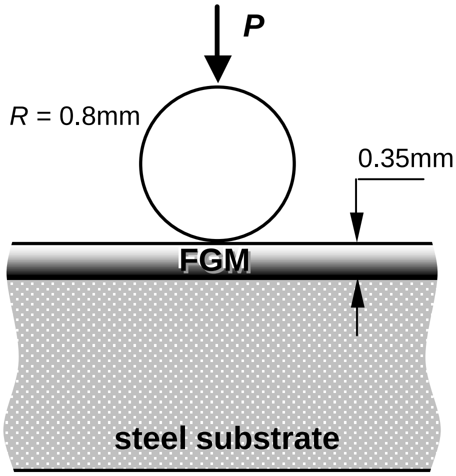

Fig. 7. Micro-indentation of FGM layer

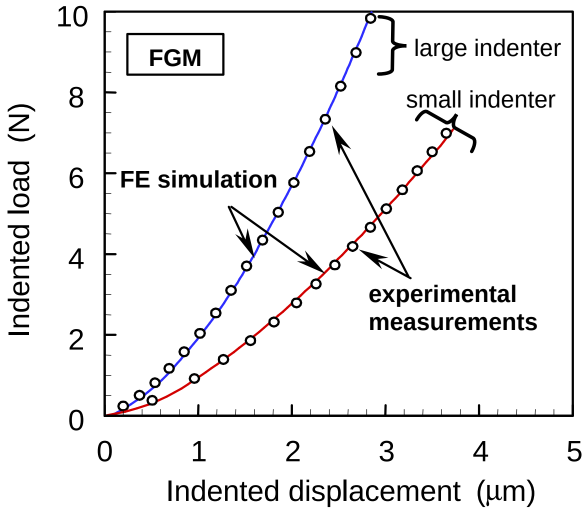

Fig. 8. Close match between the simulations and measurements when estimated properties are prescribed.

The inverse technique to determine other mechanical properties was implemented on real specimen. The graded materials composed of PSZ and NiCrAlY phases were fabricated at Stony Brook's Center of Thermal Spray Research. They were indented with instrumented micro-indentation as shown in Fig. 7. The measured indented load-displacement record was used as input for the inverse analysis and the FGM's compositional grading as well as its effective properties through thickness were determined. An excellent agreement obtained between the experimental measurements and the simulated results, shown in Fig 8, confirmed the accuracy of this technique on real FGM. The cross-section of FGM tested in shown in Fig. 9. The estimated grading from the inverse analysis and the composition obtained from a separate image analysis are shown in Fig. 10. An excellent match is observed in the results.

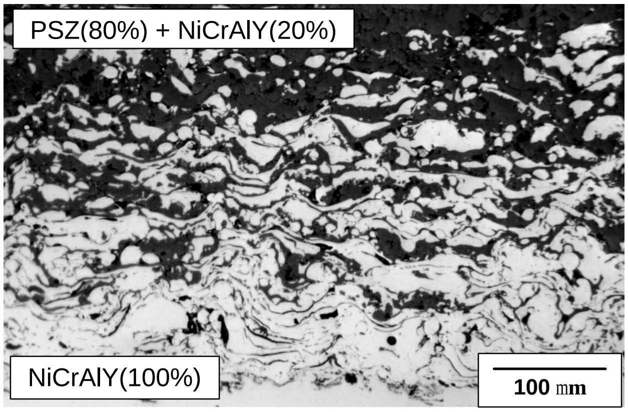

Fig. 9. Micrograph showing cross-section of thermally sprayed graded coating.

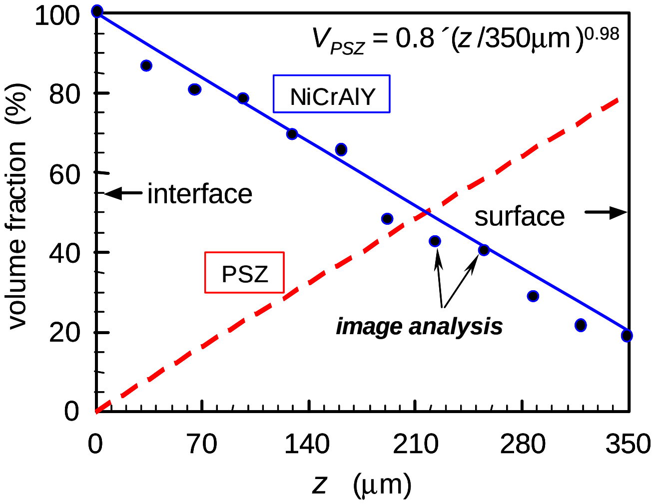

Fig. 10. Through-thickness variations of PSZ and NiCrAlY volume fractions determined from the inverse analysis. NiCrAlY variation obtained by image analysis of cross-sectional micrograph is shown with dots

A further work is underway to determine other material properties using a similar procedure. This includes fracture parameters, diffusion parameters of composites, elastic-plastic anisotropic materials. The present results based on real specimen offer promising prospects for applications of the inverse analysis to the above systems. At Stony Brook, a state of art nano-indentation system was purchased through an ARO equipment grant (DAAD19-01-1-0709) with an equal match from the State University of New York. The technique developed under this grant will be utilized for the new indenter to probe the material characteristics at nano- and micro-levels. In order to maximize extraction of accurate material information the schematic based on an inverse analysis technique, as illustrated in Fig. 11, will be carried out.

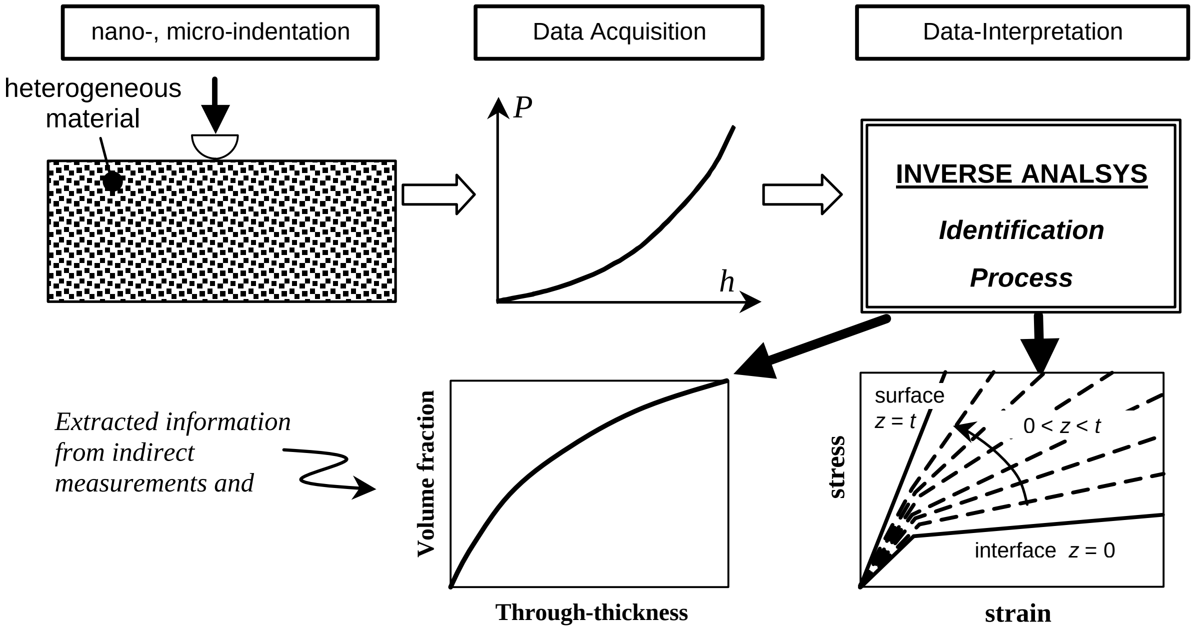

Fig. 11. Schematic of an inverse evaluation procedure with indentation measurements.

Fracture testing of read FGM for was also conducted. In collaboration with Mechanics of Advanced Materials Laboratory at Stony Brook, thick FGM specimens (t = 3~5mm) were investigated for their fracture behaviors as shown in Fig. 12. Since direct determination of any parameters which define responses of complex/heterogeneous materials is very difficult, novel data interpretation schemes based on various inverse analysis techniques are being established. Initially the fracture related parameters of FGM's are estimated from measurable record and the degradation of composite panels is estimated from surface strain measurements. As more complex materials are considered in the Army as well as advanced engineering applications, special data processing schemes to evaluate the performance of materials become more essential.

In a separate project, under partially funding of ARO, stress and failure of electronic packaging work was conducted (Gu and Nakamura, 2002). As more I/O connections are required in new generation of semiconductors, flip-chip geometry is becoming more popular.

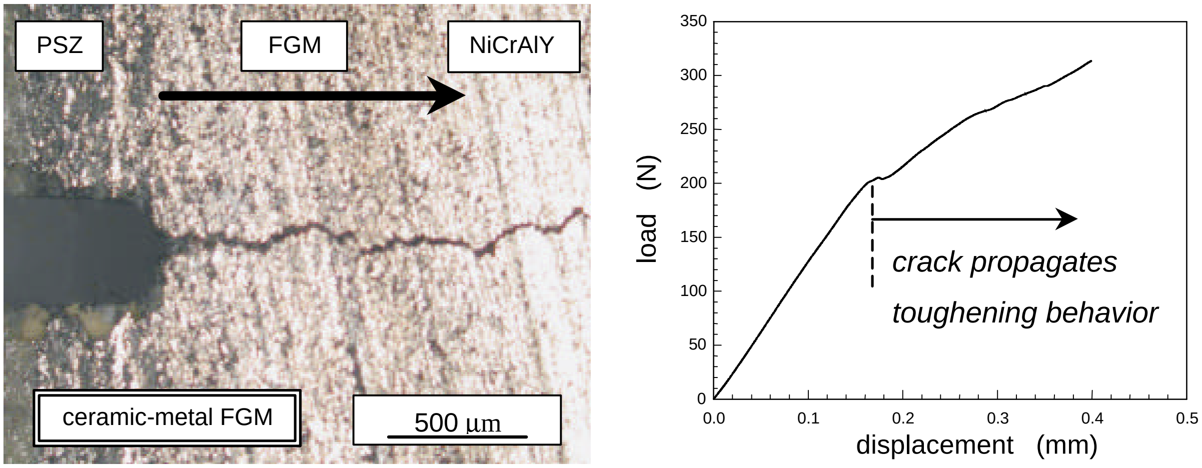

Fig. 12. Fractured FGM under three-point-bend load. The load-displacement curve shows the increasing resistance behavior as crack propagates into tougher metallic phase

In this project, detailed three-dimensional finite element analysis was carried out for area arrayed flip-chip packages. The analysis was used to quantify the three-dimensional effects on local fracture behaviors under thermal load and to estimate thermal fatigue life of solder bumps. Since dimensions of various components span more than three orders of magnitude, the multi-scale finite element model approach, were utilized to analyze the overall package deformation and the local stress and fracture characteristics near solder bumps. Here two models with different scale, global and local/cell, were adopted. The global model allows identification critical sites within the package where large deformation occurs, while the cell model represents a small region of the package that contains a single a solder bump as well as various layers of under bump metallurgies. The two-step modeling approach enabled accurate 3D investigation of interfacial delamination near solder bumps. To investigate its implication on fatigue life, the steady state cyclic shear was obtained from repeated thermal loading. The result shows about 30% greater shear in the 3D model and leads to shorter fatigue life of package than the results based on the 2D plane strain analysis.

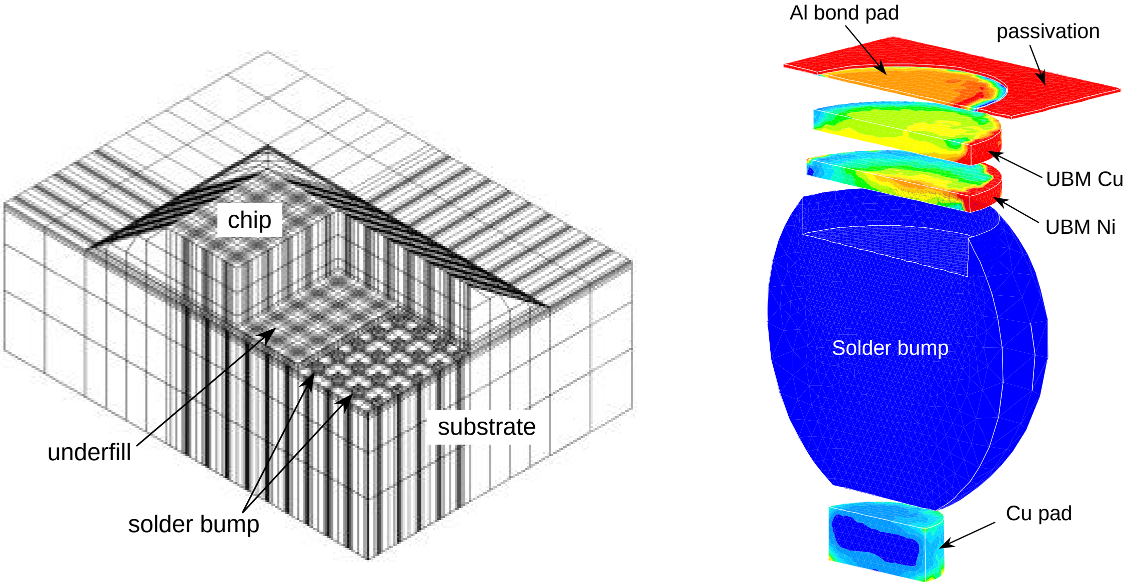

Fig. 13. 3D finite element mesh of the quarter model and detailed stress state surrounding the solder bump.

The finite element mesh and internal effective stress within the solder bump and other nearby components are shown in Fig. 13.

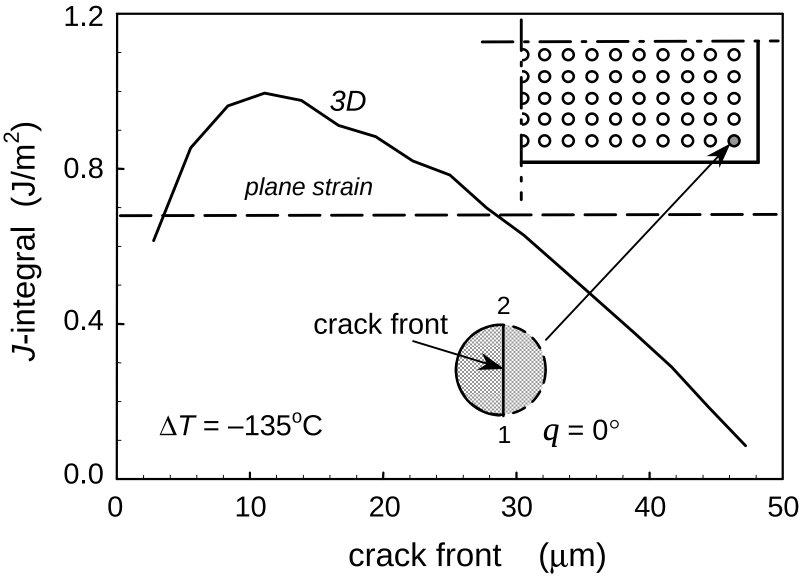

Fig. 14. Variation of *J*-integral along 3D interfacial crack front between solder bump and copper pad is shown for the $q = 0^o$ orientation (measured from 1 to 2). The solder bump location at the corner is illustrated. The peak *J* is about 40% higher than the value estimated from 2D plane strain analysis.

In the analysis, *J* along interfacial crack between the solder and copper pad was computed. It shows strong 3D effect as the embedded crack tends to propagate which may lead to loss of electrical connection. This type of facture analysis is applicable to the investigations of failures at micro-structural level where many of heterogeneous materials fail. The new procedure developed in this work can be extended many classes of materials of the Army's interest.

List of Publications and Reports

Peer-Reviewed Journals and Books

- Y. Gu, T. Nakamura, L. Prchlik, S. Sampath, and J. Wallace (2002), 'Indentation and Inverse Analysis to Characterize Elastic-Plastic Graded Materials', accepted to appear on *Materials Science and Engineering.*
- T. Nakamura and Z. Wang (2001), 'Simulations of Crack Propagation in Inhomogeneous Materials,' *Developments in Fracture Mechanics for the New Century*, eds., K. Kishimoto, S. Kubo, T. Nakamura, T. Sakagami, The Society of Materials Science, Japan, 23-32.
- T. Nakamura and S. Sampath (2001), 'Determination of FGM Properties by Inverse Analysis,' *Functionally Graded Materials 2000*, eds. K. Trumble, K. Bowman, I. Reimanis, S. Sampath, American Ceramics Society, 521-528.
- T. Nakamura and S. Sampath (2000), 'Thermally Sprayed FGM and Determination of Its Property by Inverse Analysis, *Functionally Graded Materials in 21st Century*, eds. K. Ichikawa, Kluwer Academic Publishers, 86-91.

Non Peer-Reviewed Proceedings

- T. Nakamura (2000), ‘Determination of FGM Properties using Micro-Indentation and Kalman Filter,’ *Proceedings of Symposium on the Meso-Mechanical Aspects of Material Behavior*, eds. K. Kishimoto, T. Nakamura, K. Amaya, 49-57.

Papers Presented at Conferences

- T. Nakamura, ‘Micro-Mechanical Analysis of Porous Coatings,’ (Invited), 10th International Ceramic Congress, Florence, Italy, July 2002.
- T. Nakamura, ‘Dynamic Crack Propagation in Functionally Graded Materials,’ 14th U. S. National Congress of Theoretical and Applied Mechanics, Blacksburg, VA, June 2002.
- Yu Gu and T. Nakamura, ‘3D Interfacial Delamination Near Solder Bumps in Flip-Chip Package,’ ASME 2001 IMECE, New York, November 2000.
- T. Nakamura, ‘Simulations of Crack Propagation in Inhomogeneous Materials,’ Developments in Fracture Mechanics for the New Century, JSMS 50th Anniversary Conference, Osaka University, May 2001.
- T. Nakamura, ‘Inverse Analysis to Determine FGM Properties by Micro-Indentation,’ ASME 2000 IMECE, Orlando, November 2000.
- T. Nakamura, ‘Dynamic Crack Propagation through FGM,’ Society of Engineering Science 2000, University of South Carolina, October, 2000.
- T. Nakamura, ‘Determination of FGM Properties by Inverse Analysis,’ 6th International Symposium on Functionally Graded Materials, Estes Park, Colorado, September 2000.
- ‘Determination of FGM Properties using Micro-Indentation and Kalman Filter,’ Symposium on the Meso-Mechanical Aspects of Material Behavior, Yufuin, Japan, August 2000.
- ‘Manufacturing of Thermally Sprayed FGM and Determination of its Properties by Inverse Analysis,’ (Keynote Speaker) FGMs in 21st Century by National Science and Technology Agency, Tsukuba, Japan, March 2000.

Manuscript submitted

- Z. Wang and T. Nakamura, (2002), ‘Simulations of Crack Propagation in Elastic-Plastic Graded Materials’, submitted to *Mechanics of Materials.*
- Y. Gu and T. Nakamura, (2002) ‘Interfacial Delamination and Fatigue Life Estimation of 3D Solder Bumps in Flip-Chip Packages’, submitted to *Microelectronic Reliability*.

List of Participants

Toshio Nakamura – Professor

Zhiqiang Wang – Ph.D. Graduate Student. Scheduled to complete in February 2003.

Yu Gu – Ph.D. Graduate Student. Scheduled to complete in February 2003

Bibliography

Y. Gu, T. Nakamura, L. Prchlik, S. Sampath, and J. Wallace (2002), 'Indentation and Inverse Analysis to Characterize Elastic-Plastic Graded Materials', accepted to appear on *Materials Science and Engineering.*

Y. Gu and T. Nakamura, (2002) 'Interfacial Delamination and Fatigue Life Estimation of 3D Solder Bumps in Flip-Chip Packages', submitted to *Microelectronic Reliability*.

T. Nakamura and S. Sampath (2000), 'Thermally Sprayed FGM and Determination of Its Property by Inverse Analysis, *Functionally Graded Materials in 21st Century*, eds. K. Ichikawa, Kluwer Academic Publishers, 86-91.

T. Nakamura and Z. Wang (2001), 'Simulations of Crack Propagation in Inhomogeneous Materials,' *Developments in Fracture Mechanics for the New Century*, eds., K. Kishimoto, S. Kubo, T. Nakamura, T. Sakagami, The Society of Materials Science, Japan, 23-32.

T. Nakamura and S. Sampath (2001), 'Determination of FGM Properties by Inverse Analysis,' *Functionally Graded Materials 2000*, eds. K. Trumble, K. Bowman, I. Reimanis, S. Sampath, American Ceramics Society, 521-528.

Z. Wang and T. Nakamura, (2002), 'Simulations of Crack Propagation in Elastic-Plastic Graded Materials', submitted to *Mechanics of Materials.*

Related works by other investigators are referenced in the above papers.

Appendix

The flow chart of Kalman filter implemented for the determination of unknown FGM parameters is shown below.