# REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-99-

0171



| 1. AGENCY USE ONLY *(Leave blank)* | 2. REPORT DATE | 3. REPORT TYPE AND DATES COVERED |
|---|---|---|
| | April 1999 | FINAL TECHNICAL REPORT 1 Apr 96 - 31 Mar 99 |

**4. TITLE AND SUBTITLE**
MECHANICS IN MATERIAL SPACE AND ANALYSIS OF DEFECTS

**5. FUNDING NUMBERS**
F49620-96-1-0093

61102F
2302/DX

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**8. PERFORMING ORGANIZATION REPORT NUMBER**

**9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)**
AIR FORCE OFFICE OF SCIENTIFIC RESEARCH (AFOSR)
801 N. RANDOLPH STREET, ROOM 732
ARLINGTON, VA 22203-1977

**10. SPONSORING/MONITORING AGENCY REPORT NUMBER**

**11. SUPPLEMENTARY NOTES**

**12a. DISTRIBUTION AVAILABILITY STATEMENT**
APPROVED FOR PUBLIC RELEASE, DISTRIBUTION UNLIMITED

**12b. DISTRIBUTION CODE**

**13. ABSTRACT** *(Maximum 200 words)*

The principal objective of this program was to contribute to the knowledge and understanding of complex structural degradation processes that occur in various parts of a structure, which may be subjected to a mechanical or thermal field, produced for instance, by an elevated temperature environment, or an electrical field as in piezoelectricity.

Typical degradation processes involve void and crack formation and growth, dislocation motion, as well as solid state phase transformations and chemical reactions. It is now well recognized that it is the motion, evolution and rearrangement of such defects in solids that control and determine the response of structural materials to imposed external fields. It is thus most desirable to have available an improved methodology and techniques for understanding and predicting the tendency of these imperfections to form, move and evolve, and more importantly for linking the microscale structure to the macroscale behavior of the material.

| 14. SUBJECT TERMS | 15. NUMBER OF PAGES |
|---|---|
| | 9 |
| | 16. PRICE CODE |

| 17. SECURITY CLASSIFICATION OF REPORT | 18. SECURITY CLASSIFICATION OF THIS PAGE | 19. SECURITY CLASSIFICATION OF ABSTRACT | 20. LIMITATION OF ABSTRACT |
|---|---|---|---|
| UNCLASSIFIED | UNCLASSIFIED | UNCLASSIFIED | |

FINAL REPORT

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
BOLLING AIR FORCE BASE
WASHINGTON, DC 20332-8080

For the project

# MECHANICS IN MATERIAL SPACE AND ANALYSIS OF DEFECTS

Contract #F49620-96-1-0093

For the period
April 1, 1996 to March 31, 1999

Submitted by

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April 1999

During the period of this project (1 April 1996 - 31 March 1999) major accomplishments have been achieved and the objectives of the Contract have been met.

Before stating the major accomplishments, we restate the objective of our research.

## Objective

The principal objective of this program was to contribute to the knowledge and understanding of complex structural degradation processes that occur in various parts of a structure, which may be subjected to a mechanical or thermal field, produced for instance, by an elevated temperature environment, or an electrical field as in piezoelectricity.

Typical degradation processes involve void and crack formation and growth, dislocation motion, as well as solid state phase transformations and chemical reactions. It is now well recognized that it is the motion, evolution and rearrangement of such defects in solids that control and determine the response of structural materials to imposed external fields. It is thus most desirable to have available an improved methodology and techniques for understanding and predicting the tendency of these imperfections to form, move and evolve, and more importantly for linking the microscale structure to the macroscale behavior of the material.

As an additional task, we proposed to investigate wave propagation and to study free and forced vibrations in structural elements undergoing damage.

This research is tightly related to the current and future Air Force needs. This program helps the design of high performance, yet economic, flaw-tolerant aero-space structures. It also helps deliver tools that will be used to design better composite materials and provide insight into the many options for optimizing the material to fulfill particular operational needs. Failures of structures under harsh high temperature environment are better understood and ways to reduce them were recommended. Also, methodologies to design real time health-monitoring systems are proposed.

Furthermore, the results of the supplemental task contribute to the nondestructive detection and quantification of internal damage.

## Accomplishments/New Findings

The major new findings during the span of this project may be summarized as follows.

- First, we investigated the scattering of Rayleigh (surface) waves by a sub-surface or surface-breaking crack normal to the surface. Such investigation was conducted by several authors [Achenbach and Brind, 1981; Mendelsohn et al., 1980; Visscher, 1985] who obtained numerical results for the reflection and transmission coefficients. However, due to the importance of this problem, in NDE, in correlating the scattered acoustic signal with crack characteristics, we found it necessary to derive analytical expressions for these coefficients valid in the long wavelength regime, i.e., valid for arbitrary crack depth provided the crack length is much smaller than the Rayleigh wavelength. These coefficients are related to the crack characteristics (length, depth). The scattered field generates body as well as surface waves, but only the surface waves were considered for two reasons. First the incident field itself decays exponentially with depth, and secondly, along the surface, the dominant part of the scattered wave in the far field is its surface wave component. Therefore, the scattered wave was assumed to consist of the reflected and transmitted waves. Our theory relies on Betti-Rayleigh reciprocal formula and takes into account the interference between shear and longitudinal waves. The results obtained by our method, in their region of validity and beyond, compare favorably with the numerical results of Achenbach and Brind (1981), which are themselves accurate to within 2-3%.

It was also found that the reflection and transmission coefficients of Rayleigh waves, in the long wavelength regime, are related directly to the stress intensity factors at the crack tip(s). This relationship enables one to correlate the measurements of the scattered signal not only with the size and depth of sub-surface micro-crack but also with the material strength. Such relationship has been found previously by Budiansky and Rice (1978) for scattering by body waves, but they did not investigate surface waves. Their estimate was made on the basis of the long wavelength studies by Gubernatis et al. (1977). Furthermore, the results derived under the contract for the surface wave scattering (i.e. reflection and transmission) by a single crack were formulated in such a way that they can be expanded for multiple cracks.

- Second, we derived the natural frequencies and mode shapes of a circular plate containing a small heterogeneity of arbitrary shape. Within the context of the classical theory, the solution of a circular plate with no defects can be obtained as a linear combination of the ordinary and modified Bessel functions of the first kind. Consequently, there is a significant body of literature on the subject, dealing especially with the clamped and free boundary conditions. By contrast, little work is published on the vibration of a plate in the presence of heterogeneities. Although the problem can, in principle, be solved numerically using finite or boundary element methods or finite-difference methods that handle complex geometries (e.g. the method of composite overlapping grids), it should be noted that the problem becomes progressively harder as the heterogeneities become smaller. This can be seen by considering the case of a centered circular hole of radius $\varepsilon$, the solution of which introduces the Bessel functions of the second kind, with $O(\log \varepsilon)$ singularity for the lowest mode and with increasingly higher order singularities for the subsequent modes. To circumvent this inherent difficulty, we calculated the natural frequencies and mode shapes of a circular plate with a heterogeneity through a novel approach that is based on a method of matched asymptotic expansion. This allowed us to solve for the problem when a small heterogeneity is introduced and was well suited to deal with this class of singular perturbation problems. The formulation was cast in such a way that the zeroth-order term in the outer expansion (written down in arbitrary "gauge" functions) corresponds to a certain natural frequency and associated eigenfunction of the plate with no defects. Subsequent terms were determined by enforcing solvability conditions obtained via reciprocal relations and by matching the inner and outer expansions. To confirm the asymptotic/analytical theory, a comparison of the results with those obtained for a concentric circular heterogeneity was performed. Comparison with numerical results using the finite element method was performed for other configurations.

- Third, in the area of Damage Mechanics, we laid down the foundations of a novel three-dimensional thermodynamic theory of damage in elastic solids *which takes into account thermal effects.* We showed that such a theory can be firmly based on the so-called ``Conservative or Conventional Thermodynamics of Irreversible Processes," which was first introduced by J. Meixner (1954, 1959) and I. Prigogine (1947, 1961) and elucitated in several publications by J. Kestin (1966, 1979, 1989). According to this approach, the fundamental problem on how to define and measure entropy, $S$, and thermodynamic temperature, $T$, in nonequilibrium is resolved by the introduction of the *hypothesis of local equilibrium* (HLE) also known as the *principle of local state* (PLS) (1989). This is a heuristic principle which extends the validity of the Gibbs equation into the realm of irreversible processes and leads to an explicit form for the local rate of entropy production, $\dot{\theta}$, at a point in a system which is the seat of a continuum of nonequilibrium states. This being done, the problem on how to introduce damage into the thermodynamic formulation and how to choose the variables that describe it was worked out. We argued forcefully that a `rational' selection of damage parameters *can and should* be based on the well-established concepts of equilibrium thermodynamics.

  We started by making a sharp distinction between the elastic body and the many processes that it may undergo. These processes may involve heating, straining or loading at different rates, damage evolution, etc. As a consequence of this distinction, we can state, for instance, that while the instantaneous values of the strain components may serve to characterize in part the state of the body, the strain rates describe the process and never appear in the thermodynamic potentials. We adopted Gibbs' point of view, whereby the body should be regarded as a thermodynamic system, which is characterized by extensive variables, whereas the interaction between the system and its surroundings is described by intensive variables. The values of the latter can be evaluated unambiguously at equilibrium through the equations of state. The Gibbsian phase (state) space of constrained equilibrium was described by the set of the extensive variables that can be measured in equilibrium as well as in nonequilibrium. Specifically, these consist of the internal energy, $U$, the appropriate deformation parameters such as the infinitesimal strain components, $\varepsilon_{ij}$, and the quantities associated with damage, $\alpha_k$, which *are not selected a priori but are chosen according to the form in which they enter the thermodynamic potentials.* To effect the calculation of these potentials by the traditional methods of equilibrium thermodynamics, it is necessary to imagine reversible processes (i.e., one-parameter families of equilibrium in the Gibbsian phase space) starting from an initial equilibrium state and ending in a final equilibrium state. The difficulty associated with the irreversible evolution of damage is overcome by following Bridgman's idea, which is to imagine a `Gedankenexperiment' allowing us to think that the growth or motion of the damage zones could be produced reversibly. To this end, *fictitious* conjugate forces (affinities), $A_k$, are introduced from the outside. These balance the system, as required by the postulate of reversibility, and introduce equilibrium. The irreversibility of an actual physical process of the system is due to the uncontrollable evolution of the damage parameters. These can still, however, at least conceptually, be measured in physical space and, therefore, provide a strikingly clear example of Bridgman's internal variables concept (1961). To obtain an explicit expression for the entropy production during the process, the *local-state approximation* as introduced by Meixner (1954, 1959) and Prigogine (1947, 1961) and expounded by Kestin (1966) is adopted. It was applied by associating with every nonequilibrium state an accompanying equilibrium state of equal values of $U$, $\varepsilon_{ij}$ and $\alpha_k$ and by asserting that the entropy $\overline{S}$ assignable in physical space and temperature $\overline{T}$ measured in it can be approximated by the values of $S$ and $T$ calculated in the Gibbsian phase space by the well-established methods of equilibrium thermodynamics. In this manner, an irreversible process in physical space, regarded as a continuous sequence of non-equilibrium states which can be parameterized by a single parameter, namely the time, gives rise to an accompanying reversible process in the Gibbsian state space. An explicit expression for the entropy production is then obtained by eliminating the internal energy term between the classical Gibbs equation and the energy balance equation. In order to complete the theory, empirical rate equations for the evolution of damage are needed. In the absence of such empirical relations, we proposed simple rate equations. These are subjected to the requirement of the second part of the second law of thermodynamics [Kestin, 1979], which demands that the entropy production be nonnegative. The resulting theory predicts many features of real material behavior, such as the quasi-ductility, the loading/unloading paths, the dependence of the material response on the loading or straining process (e.g., strain-rate dependency) and the transition, with the rise of temperature, from brittle to ductile behavior.

Additionally, it was found that the presence of damage modifies Fourier's law of heat conduction and makes the structure response dependent on some global geometric parameters such as the size and shape of a bar or a plate. A fact which is also confirmed by experiment.

As a further illustration of the theory, we considered the case of microcracks propagating in a one-dimensional bar and we incorporated the effect of microstructure and the associated toughening mechanism by considering a power law for the toughness curve ($K^R$-curve). The stress-strain curves obtained were then compared with experimental results performed on alumina specimens and an excellent quantitative agreement was obtained between theory and experiment.

- Fourth, a monograph on the Mechanics in Material Space has been prepared. It presents for the first time in print form the new field, which was termed by the first author of this report "Mechanics in Material Space" (MiMS}. It draws analogies between this heretofore unexplored field and the traditional Newtonian Mechanics, which may be named "Mechanics in Physical Space" (MiPS), with view towards applications to defects and crack mechanics. It presents three methods for deriving conservation laws, including the new Neutral Action Method, which was derived with AFOSR support. Applications to homogenous and heterogeneous beams, plates and shells along with applications to dissipative systems, such as thermoelasticity are presented. Furthermore, the elements of Eshelby tensor of defect mechanics are explored in detail and are given physical interpretation.

- Fifth, we studied the properties of Eshelby's tensor and we proposed novel methods based on the concept of virtual work, to derive each of its components thus yielding a new physical interpretation of this important tensor. A paper summarizing these results was published (Kienzler and Herrmann). Also, a monograph on the same subject was written. Separately, using the results of the methodology of heterogenization described below, we calculated the attractive and repulsive "configurational" forces acting between two circular inclusions (fibers) when the matrix material is subjected to arbitrary antiplane loading. The regions of attraction and repulsion on a fiber where drawn in terms of the position of the fiber for a given configuration (position of another fiber) and loading of the matrix. Furthermore, the interaction of these fibers with microdefects (e.g., dislocations) was scrutinized. A paper describing these results is in press (E. Honein et al.).

- Sixth, conservation laws in nonhomogeneous elastostatics were studied by means of a special version of Noether's theorem on invariant variational problems. The investigation was restricted to isotropic, linearly elastic bodies with smoothly varying elastic moduli and subjected to plane strain deformation fields. By applying Lie's infinitesimal criterion on the invariance of the action integral under a continuous transformation group, it was found that the materials admitting conservation laws are those for which the elastic parameters satisfy a first order linear partial differential equation. While the general solution to this equation is readily available, a special emphasis was placed on extending Rice's J-integral to certain class of materials with varying Young's modulus in the direction of a crack line. The extended integrals are related to stress intensity factors at the crack tip, and their use was illustrated by applying them to two simple examples. Also, the circumstances under which these integrals can be generalized to three-dimensional case were briefly discussed. A paper describing these results was published (T. Honein and G. Herrmann).

- Seventh, in the area of Heterogenization we calculated the effects of the presence of a fiber embedded in a matrix material on the distribution of the thermomechanical field. The effect of the interfaces on the microbehavior of a composite material system under thermoelastostatic loading was also investigated. We also studied the interaction of two fibers embedded in a matrix and subjected to arbitrary loadings that give rise to two dimensional elastic field. A paper dealing with this topic is in press (E. Honein et al.).

Also, the plane elasticity problem of two circular inclusions of distinct radii, occupied by two different materials and perfectly bonded to a matrix that is subjected to arbitrary loading or singularities has been solved analytically. Using the heterogenization methodology, the problem was cast into the form of functional equations relating the values of functions and their derivatives at distinct points and allowing the extraction of useful information. In particular, universal formulae are obtained for the average stress between two holes. It was shown that two holes approaching each other give rise to crack-type singularity. These results shed new light on the interaction of defects at both the microscale and macroscale level and highlight the inadequacy of current methodologies based on effective property concept in dealing with such problems.

Finally, discrepancies between experimental and theoretical predictions based on linear piezoelectric crack models have been addressed. It was suggested that nonlinear electric behaviors of piezoelectric solids may play a more important role than previously expected. A "strip saturation" model has been proposed in which electrical polarization is assumed to reach a saturation limit in a line segment in front of a crack. Two energy release rates emerge from this model. An "apparent" or global energy release rate appears when evaluating $J$-integral along a contour surrounding both the electrical yielding strip and the crack tip. A "local" energy release rate is obtained by evaluating $J$ along an infinitesimal contour near the crack tip. The strip saturation model has been solved using a simplified electroelasticity formulation in which only three material constants and two degrees of freedom are considered; the local energy release rate has been shown to give predictions which are in broad agreement with experimental observations. One of the interesting results coming out of the simplified analysis is that the mechanically singular local crack-tip field and the local energy release rate are independent of electric yielding parameters such as the yield strength and the yield zone size. The validity of this statement in a more general setting has been proved to remain true. These results have been detailed in a paper published in the Journal of the Mechanics and Physics of Solids and in a separate note published in the International Journal of Fracture (H. Gao et al.).

- Finally, in the area of piezoelectricity, fundamental study on the effect of defects/damage on wave propagation in piezoelectric layered media is being conducted. We started by developing a one-dimensional model of wave propagation in multilayered piezoelectric materials. A new formulation, based on a matrix Riccati equation and valid when inhomogeneities are present, is being used. This formulation is numerically stable for all frequency ranges. A recovery scheme which permits the computation of the state vector directly from the surface impedance matrix and the entries of the fundamental piezoelectric matrix is being exploited. A software package is being developed to calculate the reflected signal during the thickness and the material properties of all layers. The effect of defects will be characterized. The interface will be evaluated. The formulation will be extended to three dimensions. A mixed representation will be developed that enables us to solve the problem using numerical schemes such as the finite element method or the boundary element method.

## Personnel Supported

- Professor George Herrmann
- Professor Huajian Gao
- Dr. Elie Honein, Research Associate
- Lin Zhang, Graduate Student

## Publications


1. R. Kienzler and G. Herrmann, 1997, "On the Properties of Eshelby Tensor," *Acta Mechanica*, **125**, pp. 73-91.
2. E. Honein et al., "Energetics of Two Circular Inclusions in Anti-Plane Elastostatics", *Int. J. Sol. Struct.,* in press.
3. T. Honein and G. Herrrmann, 1997, "Conservation Laws in Non-Homogeneous Plane Elastostatics," *J. Mech. Phys. Solids.,* **45**, pp. 789-805.
4. E. Honein and G. Herrmann, "Approximate Analysis of Surface Wave Scattering by a Surface-Breaking or Sub-Surface Crack," to be submitted for publication.
5. E. Honein et al., "A Physically-Based Theory of Damage Accumulation in Elasto-Plastic Materials Incorporating the Effect of Microstructure," presented in November 1998, Boston.
6. E. Honein et al., "Two Circular Inclusions in Plane Elastostatic," submitted for publication.
7. T. Honein et al., "A Novel Thermodynamic Theory of Damage in Elastic Solids and the Effect of Microstructure on the Stress-Strain Curves," to be submitted for publication.
8. T. Honein et al., "The Elements of A Thermodynamic Theory of Nonisothermal Damage in Elastic Solids," to be submitted for publication.
9. G. Herrmann and R. Kienzler, *Mechanics in Material Space with Application to Defects in Fracture Mechanics,* monograph in press.
10. H. Gao and D.M. Barnett, 1996, "An Invariance Property of Local Energy Release Rates in a Strip Saturation Model of Piezoelectric Fracture," *Int. J. Fracture*, **79** No. 2, pp. R25-9.
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Euler's Buckling formulas, which was 250 years old in 1994 and review of further developments during the last 50 years).

14. N. Chien and G. Herrmann, "Conservation Laws for Thermo or Poroelasticity," *J. Appl. Mech.*, **63**, pp. 331-336, June 1996.

## New Discoveries, Inventions, or Patent Disclosures

None

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