FINAL REPORT

"ENERGY CHANGES IN TRANSFORMING SOLIDS"

JANUARY 31, 1991 to JANUARY 31, 1995

PROJECT # ENERGY DE -FG03-87ER13662

submitted to the U.S. DEPARTMENT OF ENERGY

OFFICE OF BASIC ENERGY SCIENCES

DIVISION OF MATHEMATICAL AND GEOSCIENCES

(attn: DR. OSCAR P. MANLEY)

SUBMITTED BY:

***PROFESSOR GEORGE HERRMANN (CO-P.I.)**

****PROFESSOR DAVID M. BARNETT (CO-P.I.)**

April 3, 1995

***Division of Applied Mechanics
Stanford University
Stanford, CA. 94305**

****Department of Materials Science & Engineering
Stanford University
Stanford, CA. 94305-2205**

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

FINAL REPORT ENERGY CHANGES IN TRANSFORMING SOLIDS

Professor George Herrmann

In this part of the project we proceeded along three lines. Firstly, we developed a new thermodynamical theory of continuum damage mechanics capable of incorporating non-isothermal processes and of providing explicit expressions for the thermal dissipation during damage evolution. Secondly, we further advanced the recently developed methodology of heterogenization to analyze elastic bodies with inclusions and defects, and we implemented new approaches to study the behavior of multiphase and modern composite materials. Finally, we applied the newly proposed *Neutral Action* method to derive conservation laws and path-independent integrals for non-homogeneous and dissipative systems.

The recently formulated thermodynamic theory of elastic bodies prone to damage is based on classical thermodynamics in the form of the local state approximation. The parameters needed to specify the damage are treated as internal variables in the sense of Bridgman. Some concepts have been clarified by invoking Onsager's reciprocal relations. The theoretical results obtained agree quite well with existing experimental results.

We extended and applied the methodology of *heterogenization* to problems in elasticity, thermoelasticity, and piezoelectricity. Novel concepts pertaining to Kelvin and Möbius transformations, with their associated iterations and fixed points, group theory, linear operators in Banach spaces, inductive schemes, discontinuous groups, and automorphic functions were employed.

As regards conservation laws, we have applied the *Neutral Action* method to various systems of practical interest, including thermoelastic, porous, and piezoelectric media. Our results fall into two categories, namely, conservation laws in physical space and in material space. In physical space the results obtained are alternative formulations of the governing equations; in general, these results do not offer new insight into the behavior of the systems studied. In material space, however, our results can often be expressed in forms parallel to the path-independent integrals associated with linear elasticity, and they will prove useful in the analysis of fracture and defects in such systems. In particular, for thermo- and poro-elasticity, we have shown that the analogous J-integral obtained is a representation of the energy release rate accompanying crack extension in a thermo- or a poro-elastic medium. Due to path-independence, this conservation integral is truly an extension of the classical J-integral for the dissipative thermoelastic and poroelastic media.

The reprints and preprints of manuscripts stemming from Professor Herrmann's portion of research supported by this grant are enclosed with this report and are listed as publications 1 through 16 under *Publications*.

Professor David M. Barnett

We began an investigation of two problems involving bonded dissimilar piezoelectric half-spaces, one a static problem and the other a dynamic one. An asymptotic analysis of interfacial cracks in joined piezoelectric half-spaces was performed for various combinations of mechanical and electrical boundary conditions on the upper and lower crack faces (the crack can be taken as semi-infinite for purposes of an asymptotic analysis whose goal is to extract the field singularities at the crack tip). This particular analysis forms the basis for a fracture mechanics framework for interfacial cracks in bonded piezoelectrics. The dynamic problem studied was an examination of conditions permitting interfacial or Stoneley waves in bonded piezoelectrics.

Simultaneously a short study was initiated to develop a computer graphics routine capable of yielding three-dimensional views of slowness surfaces for anisotropic crystals. Such graphical information lets the investigator make a better guess at which crystal directions may yield interesting wave phenomena in anisotropic media. A more pithy examination was initiated to determine if **one-component** surface waves are possible in anisotropic half-spaces (Usually three partial waves are needed for surface wave construction, although if the reference plane is a symmetry plane, only two partial waves are required). We had already decided that an earlier proof by Chadwick discounting the existence of such one-component waves was in error, so that a fresh examination of the issue was warranted.

The above-mentioned 4 problems had been studied and published by mid-1991. Since the one-component surface wave problem had indeed turned out to be a possibility and had turned out to be supersonic and polarized parallel to the free surface, we thought it prudent to inquire as to whether a two-component subsonic surface wave could ever exist with its polarization parallel to the free surface. The answer turns out to be no, although lifting the restriction of subsonic gives rise to such waves. By late 1991 we had also completed a somewhat exhaustive study of the conditions giving rise to so-called Type 3 first transonic states in anisotropic elastic crystals (The Type 3 state was one of the two remaining ordinary transonic states not yet found in real crystals). We were able

to rigorously show that for isotropic, hexagonal, tetragonal, trigonal, and cubic symmetry, only hexagonal and tetragonal symmetry admit such states; relations between the elastic stiffnesses admitting such states were derived.

The newest graduate student on this project, Albert Lavagnino, began to work on two portions of his dissertation project in 1991. His first project, now completed, involved studying a material of no symmetry (i.e., triclinic symmetry) whose elastic constants are such as to admit a supersonic one-component surface wave. For the same geometry admitting the one-component surface wave, a state of **simple reflection** must also exist according to the general theory developed by Alshits and Lothe in 1979. Lavagnino has found that surrounding this geometry are other states of simple reflection and other supersonic surface waves, i.e., the one-component surface wave is not an isolated point in slowness space. This part of the project has been an intensive numerical study requiring, among other things, finding a way to deal numerically with matrices which exhibit non-semisimple degeneracy. Our final study of waves in anisotropic media was concerned with interfacial waves in bonded "piezo-crystals", i.e., bonded half-spaces exhibiting piezoelectric, piezomagnetic, and elastic properties. This study delineated the number and types of "piezo-" Stoneley waves possible for different interfacial boundary conditions.

Following work by Ting and Barnett, we returned to the problem of straight dislocations in bimetals studied in isotropic solids many years ago by Dundurs and Sendeckyj and in anisotropic media by Barnett and Lothe in 1974. These problems are of modern technical interest as models of defects near interfaces in thin film/substrate systems and in composite materials. Dundurs and Sendeckyj found, quite correctly, that a pure edge dislocation in an isotropic bimetal would usually be repelled from one side of the interface and attracted toward the interface from the other side; it is possible that "mutual repulsion" or repulsion from both sides of the interface may occur for certain combinations of the elastic constants (actually of the Dundurs' parameters α and β), but they found that "mutual attraction" is not possible. We have shown that "mutual attraction" is possible in an isotropic bimetal if the dislocation is of **mixed** character, i.e., if it has both edge and screw character, and have delineated the restrictions on the elastic constants allowing mutual attraction. This work was presented at the Dundurs Symposium at the Twelfth U.S. National Congress on Applied Mechanics in June, 1994 (Seattle).

A natural extension of the "mutual attraction" problem is to see to what extent mutual attraction and mutual repulsion are possible in bonded dissimilar half-spaces of

arbitrary anisotropy. This was a second topic of investigation by Lavagnino; it is obviously a difficult problem if only because of the many possibilities introduced by anisotropy and bimaterial combinations. We have been able to show that if the stiffnesses of the two media are proportional, then neither mutual attraction nor mutual repulsion can occur. In order to see under what conditions mutual attraction or repulsion might exist, we have initially set the problem in a simpler context, namely two initially identical anisotropic half-spaces which are then misoriented relative to one another by an infinitesimal relative rotation about the interface normal. First order perturbation theory shows that neither mutual attraction nor repulsion can occur unless the first order variation vanishes identically. For any interface, it turns out there is always a dislocation line direction and Burgers vector for which this is possible. Second order perturbation theory appears to open up mutual repulsion and perhaps mutual attraction possibilities. This work is currently being written for publication. We should probably add that these issues of "mutual attraction" or "mutual repulsion" are very topical given the amount of effort devoted by modern materials scientists to cross-section transmission electron microscopy observations of misfit dislocations in thin film systems and modeling to explain these observations.

The last part of Lavagnino's thesis has been completed and is concerned with the development of a fast algorithm for numerically computing the three-dimensional anisotropic elastic Green's functions and their derivatives, as would be required in anisotropic elastic 3-D boundary integral equation methods. We believe the algorithm generated is the most efficient and most accurate method proposed to date for numerical computation of the 3-D tensor elastic Green's functions for anisotropy.

The method of attack used in most of the problems described above involves extensions of the so-called Stroh formalism for plane anisotropic problems, a formalism which we have help to extend under DOE support (In a book on anisotropic elasticity emphasizing the Stroh formalism and due to appear within about a year, T. C. T. Ting refers to three of the basic tensors of this theory as the Barnett-Lothe tensors). The publications emanating from Professor Barnett's portion of this research are listed under *Publications* beginning with publication #17.

PUBLICATIONS

Professor George Herrmann

1. T. Honein, N. Chien, and G. Herrmann, "On Conservation Laws for Dissipative Systems", **Physics Letters A**, v. 155, nos. 4 & 5, pp. 223-224 (1991).
2. H. Gao and G. Herrmann, "On Estimates of Stress Intensity Factors for Cracked Beams and Pipes", **Engineering Fracture Mechanics**, v. 41, no. 5, pp. 695-706 (1992).
3. E. Honein, T. Honein, and G. Herrmann, "On Two Circular Inclusions in Harmonic Problems", **Quarterly of Applied Mathematics**, v. L, no. 3, pp. 479-499 (1992).
4. W. H. Müller, G. Herrmann, and H. Gao, "Elementary Strength Theory of Cracked Beams", **Theoretical and Applied Fracture Mechanics**, v. 18, pp. 163-177 (1993).
5. N. Chien, T. Honein, and G. Herrmann, "Conservation Laws for Linear Viscoelasticity", **Zeit. Angew. Math. Phys.**, v. 44, pp. 44-52 (1993).
6. W. H. Müller, G. Herrmann, and H. Gao, "A Note on Curved Cracked Beams", **International Journal of Solids and Structures**, v. 30, no. 11, pp. 1527-1532 (1993).
7. T. Honein, B. V. Honein, E. Honein, and G. Herrmann, "On the Interaction of Two Piezoelectric Fibers Embedded in an Intelligent Material", in **Adaptive Systems and Material Structures**, eds. G. P. Carman and E. Garcia, AD-Vol. 45, Book No. H00873, ASME, pp. 105-112 (1993).
8. N. Chien, T. Honein, and G. Herrmann, "Conservation Laws for Nonhomogeneous Bernoulli-Euler Beams", **International Journal of Solids and Structures**, v. 30, no. 23, pp. 3321-3335 (1993).
9. T. Honein, E. Honein, and G. Herrmann, "Circularly Cylindrical and Plane Layered Media in Antiplane Elastostatics", **Journal of Applied Mechanics**, v. 61, pp. 243-249 (1994).
10. E. Honein, T. Honein, and G. Herrmann, "Aspects of Heterogenization", **Journal of Engineering Materials and Technology**, v. 116, pp. 298-304 (1994).
11. T. Honein, E. Honein, and G. Herrmann, "A Thermodynamically Based Theory of Damage in Brittle Structures", in **Fracture and Damage in Quasi-brittle Structures**, eds. Z. P. Bazant, Z. Bittnar, M. Jirasek, and J. Mazars, pp. 86-98, Boundary Row, London, UK (1994).
12. G. Herrmann, "Micromechanics: Some Basic Methods and Current Trends", in **Micromechanics of Concrete and Cementitious Composites**, ed. C. Huet, pp. 1-18, Presses Polytechniques et Universitaires Romandes, Lausanne (1993).

13. N. Chien, T. Honein, and G. Herrmann, "Conservation Laws for Nonhomogeneous Mindlin Plates", **International Journal of Engineering Science**, v. 32, no. 7, pp. 1125-1136 (1994).
14. E. Honein, T. Honein, and G. Herrmann, "Further Aspects of the Elastic Field for Two Circular Inclusions in Antiplane Elastostatics", **Journal of Applied Mechanics**, v. 59, pp. 774-779 (1992).
15. E. Honein, T. Honein, and G. Herrmann, "Stress Analysis of Functionally Gradient Materials Based on a Heterogenization Procedure", to appear in FGM '94, Lausanne, Switzerland.
16. N. Chien, H. Gao, G. Herrmann, and D. M. Barnett, "Diffusive Surface Instabilities Induced by Electromechanical Loading", under review for **Proceedings of the Royal Society, London**.

Professor David M. Barnett

17. Abbudi, M. and Barnett, D. M., On the Existence of Interfacial (Stoneley) Waves in Bonded Piezoelectric Half-Spaces, **Proceedings of the Royal Society, London**, A429, pp. 587-611 (1990).
18. Gao, H., Abbudi, M. and Barnett, D. M., Interfacial Crack Tip Fields in Anisotropic Elastic Solids, **Journal of the Mechanics and Physics of Solids**, 40, #2, pp. 393-416 (1992).
19. Barnett, D. M., Chadwick, P. and Lothe, J., The Behaviour of Elastic Surface Waves Polarized in a Plane of Material Symmetry. I. Addendum, **Proceedings of the Royal Society, London**, 433, pp. 699-710 (1991).
20. Suo, Z., Kuo, C-M., Barnett, D. M. and Willis, J. R., Fracture Mechanics for Piezoelectric Ceramics, **Journal of the Mechanics and Physics of Solids**, 40, #4, pp. 739-765 (1992).
21. Kuo, C-M. and Barnett, D. M., Stress Singularities of Interfacial Cracks in Bonded Piezoelectric Half-Spaces, in **Modern Theory of Anisotropic Elasticity and Applications**, eds. Wu, J. J., Ting, T. C. T. and Barnett, D. M., pp. 33-50, SIAM, Philadelphia (1991).
22. Barnett, D. M. and Chadwick, P., The Existence of One-Component Surface Waves and Exceptional Subsequent Transonic States of Types 2, 4, and E1 in Anisotropic Elastic Media, in **Modern Theory of Anisotropic Elasticity and Applications**, eds. Wu, J. J., Ting, T. C. T. and Barnett, D. M., pp. 199-214, SIAM, Philadelphia (1991).
23. Abbudi, M. and Barnett, D. M., Three-Dimensional Computer Visualization of the Slowness Surfaces of Anisotropic Crystals, in **Modern Theory of Anisotropic Elasticity and Applications**, eds. Wu, J. J., Ting, T. C. T. and Barnett, D. M., pp. 290-300, SIAM, Philadelphia (1991).
24. Barnett, D. M., On the Non-Existence of Subsonic Boundary Polarized Two-Component Surface Waves, in **Statistical Physics, Elasticity and Dislocation**

Theory, Festschrift in honor of Jens Lothe on his 60th birthday (November 25, 1991), eds. Jossang, T. and Barnett, D. M., pp.225-240, the University of Oslo, Oslo, Norway (1991). Also in *Physica Scripta*, vol. T44, pp. 98-103 (1992).

25. Barnett, D. M. and Lothe, J., Conditions Admitting the Existence of Type 3 Transonic States in Stable Anisotropic Linear Elastic Media, **Journal of the Mechanics and Physics of Solids**, **40**, #7 (Elastic Waves and Related Topics, Papers from the Conference held in honor of Peter Chadwick, F.R.S.; edited by J. R. Willis), pp. 1433-1448 (1992).
26. Ting, T. C. T. and Barnett, D. M., Image Force on Line Dislocations in Anisotropic Elastic Half-Spaces With a Fixed Boundary, **International Journal of Solids and Structures**, **30**, #3, pp. 313-323 (1993).
27. Barnett, D. M. and Lothe, J., "Mutual" Attraction of a Dislocation to a Bi-Metallic Interface and a Theorem on "Proportional " Anisotropic Bi-Metals", **International Journal of Solids and Structures: Special Topics in the Theory of Elasticity - A Volume in Honor of Professor John Dundurs**, v. **32**, #3/4, pp. 291-302 (1995).
28. Alshits, V. I., Barnett, D. M., Darinskii, A. and Lothe, J., On the Existence Problem for Localized Acoustic Waves on the Interface Between Two Piezocrystals, **Wave Motion**, **20**, #3, pp. 233-244 (1994).