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From: J.K. Knowles and R. Abeyaratne

Subject: Final Report for ONR Contract N00014-87-K-0117 with California Institute of Technology entitled "Investigations of Non-elliptic Elastic Materials and the Modeling of Dissipative Behavior in Solids"

We summarize below the research goals and accomplishments associated with the above contract. We also list those who have participated in the research, and we list the technical presentations made by the investigators.

1. Research Goals. Our efforts have been directed primarily at the study of non-elliptic elastic/thermoelastic materials. Such materials are capable of sustaining equilibrium deformations with discontinuous deformation gradients, and because of this, they provide a natural setting for the modeling within continuum theory of certain kinds of phase transformations in solids. Examples include martensitic phase transformations of the kind occurring in shape-memory alloys. In particular, non-elliptic elastic materials are appropriate for the description of isothermal processes such as quasi-static motions involving slowly moving surfaces of strain discontinuity. Such motions are dissipative in the sense that, for any portion of the body, the rate of work of the external forces differs from the rate of storage of strain energy. This energy imbalance allows one to introduce the notion of a "driving traction" - or "Eshelby force"- acting on the moving surface of discontinuity, i.e. "phase boundary". This in turn permits one to model the kinetics and nucleation of phase boundaries as the body evolves quasi-statically through metastable states. The first goal of the research performed under the above contract was to investigate the extent to which such modeling is possible in a purely mechanical context, and whether it yields results in qualitative accord with experiments involving slowly moving phase boundaries.

Our second goal was to explore the extent to which non-elliptic elastic materials provide models applicable to "fast" phase transitions of the kind that are known to occur in some alloys. In this situation, inertial effects must be taken into account.

The third goal of the research carried out under the contract was to account for thermal as well as mechanical effects in thermoelastic materials, both for slow phase transitions and for those involving inertia.

2. Research Results. Our earliest efforts were devoted to two aspects of the general issue: (i) the study of fundamental properties of non-elliptic elastic materials, and (ii) the elucidation of mechanical phenomena that can be modeled by such materials. As regards fundamental properties, the principal results were summarized in [1,2]*. The first of these completely characterizes the structure of strain discontinuities and the associated driving traction for plane deformations of homogeneous, isotropic, incompressible non-elliptic elastic materials. The analysis in [2] represents a major clarification of the theory of three-dimensional finite deformations of non-elliptic elastic materials. Based on a new kinematic decomposition developed expressly for the task at hand, the results in [2] furnish a clear physical interpretation of the conditions under which the governing equilibrium differential equations of finite elasticity lose ellipticity. This interpretation leads to improved understanding of the conditions under which equilibrium deformations exist in which the strains are discontinuous.

Having shown in [3,4] that macroscopic mechanical phenomena similar to those associated with elastic-plastic behavior can be modeled with the help of non-elliptic elastic materials, we turned in [5,6] to the modeling of quasi-static behavior in one-dimensional nonlinearly elastic bars with non-monotonic stress-strain relations; such bars support quasi-static processes with stain discontinuities. In [6] it was shown that the macroscopic response of bars of this kind can mimic that of viscoelastic tensile specimens. In [5], we viewed the theory of bars as modeling slow solid-solid phase transitions, and we showed that the theory required additional constitutive information pertaining to the nucleation and evolution of the phase transformation if it was to lead to a determinate macroscopic response. When such additional information is supplied, the theory leads as shown in [5] to hysteretic force-elongation behavior qualitatively similar to that found in experiments such as those reported in [7].

Another physical phenomenon to which the theory of non-elliptic elastic materials is applicable is that of "transformation toughening" against fracture in ceramics by the addition of second-phase particles that exhibit dilatational phase transformations. The pilot transformation-toughening problem treated in [8,9] involves a hollow sphere composed of a nonelliptic elastic material capable of undergoing solid-solid phase transitions that is subject to uniform tension on its outer surface, the inner surface remaining free. As the load is slowly increased, the analysis predicts a sudden drop in stress concentration at the instant when the phase transformation is initiated. This is a manifestation of the increased toughness associated with such materials. As in the theory of bars described above, the need for a nucleation criterion and a kinetic relation for the phase transition is needed here as well. The analysis in [8,9] is carried out in the "small-strain, constitutively nonlinear" setting.

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* Numbers in brackets refer to the references listed at the end of this report.

Our first efforts to include thermal effects as well as mechanical ones in the continuum modeling of solid-solid phase transitions are represented by the work reported in [10-12]. Because the notion of the driving traction at a phase boundary (or strain discontinuity) had played a central role in our earlier work, we felt it important to determine whether this concept survives when thermal effects are considered and when the elastic constitutive law is relinquished. In [11] we analyzed the motion of a strain discontinuity in an arbitrary continuum in three dimensions, with both inertial and thermal effects taken into account, and we showed that the notion of driving traction at such a singular surface has thermomechanical significance in the absence of any constitutive law whatsoever. In [11] we also give further thermodynamic arguments in support of the need to introduce into the continuum theory a kinetic relation, a concept that has long been recognized in materials science as crucial for the understanding of phase transitions.

Thermodynamic considerations of the kind reported in [11] form the basis for the work undertaken in [12], where a thermoelastic model is developed for materials of the "shape-memory" type. Included in [12] is an analysis of quasi-static thermomechanical solid-solid phase transitions in anti-plane shear. This analysis is applied to the qualitative prediction of the transformation-induced creep observed in an experiment reported in [13] and motivated by a geological issue concerning possible phase transformations in the earth's mantle. The model in [12] does indeed predict the qualitative features of this experiment. The detailed constitutive model used in [12] makes use of a hypothetical material described in [10].

The third major thrust of our research during the contract period concerned the extension to genuine dynamics of the continuum model of phase transitions including the nucleation criterion and the kinetic relation governing the respective initiation and evolution of solid-solid phase transitions. Since such transitions have been observed experimentally in some materials to involve phase boundaries moving at speeds approaching a shear wave speed of the material [14], such a dynamical theory would be physically relevant. Moreover, if the nucleation criterion and the kinetic relation are indeed truly constitutive in character, as assumed in our quasi-static theory, it must be possible to include them in a theory that accounts for inertial effects. In [15], we have presented a study of rapidly propagating phase boundaries in one-dimensional tensile bars, emphasizing the question of whether the nucleation criterion and kinetic relation are compatible with the dynamical theory of bars. This is an issue of some subtlety, since propagating discontinuities may now be either shock waves or phase boundaries. Nucleation and kinetics, if applicable at all, should be necessary only at the latter, and not permissible at the former. For a special nonlinearly elastic material, the analysis in [15] confirms that a nucleation criterion and a kinetic relation are indeed required and can be accommodated in the simplest continuum theory of the dynamics of tensile bars.

Various alternative approaches to problems involving rapidly propagating phase boundaries have been proposed in the literature*. In one of these, the elastic constitutive law is modified by adding to the elastic part of the stress effects due to viscosity and second strain gradient. One then declares propagating phase boundaries in the purely elastic theory to be admissible if they can be obtained from traveling waves in the augmented theory in the limit of zero viscosity and zero strain gradient effect. In [16], we have compared this approach to dynamically propagating phase boundaries with the one developed in [15] that involves nucleation criteria and kinetic relations. We have shown in [16] that the viscosity-strain gradient theory is equivalent to our theory, provided a suitable special choice of the kinetic relation is made in the latter.

Finally, we note that two small, four-day informal workshops on phase transformations and finite elasticity were organized by R. Abeyaratne and held in South Pomfret, Vermont, during the summers of 1989 and 1990. About a dozen experts attended; one-hour lectures were followed by unlimited discussion, and the workshops were indeed very stimulating.

3. List of Participants. Those who took part in the research supported by the contract are:

J.K. Knowles, Professor of Applied Mechanics, Caltech;

R. Abeyaratne, Associate Professor of Mechanical Engineering, MIT;

E. Fried, graduate student, Caltech;

G.H. Jiang, graduate student, MIT;

Q. Jiang, graduate student, Caltech;

Y. Lin, graduate student, MIT;

M. Lusk, graduate student, Caltech;

P. Rosakis, graduate student, Caltech.

P. Rosakis received the Ph.D. degree from Caltech in June, 1989, and he is now on the faculty in the Department of Theoretical and Applied Mechanics at Cornell University. G.H. Jiang received the Ph.D. from MIT in February, 1990, and he is now employed at the Ford Motor Company. Q. Jiang received the Ph.D. from Caltech in June, 1990, and he will join the faculty in the Department of Engineering Mechanics at the University of Nebraska in August, 1991. E. Fried received the Ph.D. from Caltech in June, 1991, and he will take up a post-doctoral position in the Department of Mathematics at Carnegie Mellon University immediately.

M. Lusk and Y. Lin are expected to complete the requirements for their Ph.D.'s in June, 1992.

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* See the references in [15].

4. Presentations. During the contract period, the various participants gave invited presentations as follows:

R. Abeyaratne: Departmental seminars at Brown University, Harvard University, University of Minnesota, Texas A&M University, University of Texas at Austin, University of Houston, University of Pittsburgh, Michigan State University, Cornell University, Johns Hopkins University; lecture at the Workshop on the Reliability of the Finite Element Method, University of Maryland; lecture at the 11th U.S. National Congress of Applied Mechanics, Tucson; lecture at the Workshop on Shock Induced Transitions and Phase Structures in General Materials, Institute of Mathematics and its Applications, University of Minnesota.

J.K. Knowles: Departmental seminars at Tsing Hua University and the Beijing University for Aero- and Astronautics in Beijing, University of California at San Diego, Brown University, Cornell University, University of Minnesota; lecture at International Conference on Fracture and Fracture Mechanics, Shanghai; lecture at Greek National Congress of Mechanics, Athens; symposium lectures, ASME Winter Annual Meetings, San Francisco in 1989 and Dallas in 1990.

Q. Jiang: Departmental seminars at the University of Manitoba, the University of Western Ontario, Stanford University and the University of Nebraska.

P. Rosakis: Departmental seminars at Stanford University, Cornell University, Brown University and MIT.

In addition, a contributed paper was given by Abeyaratne and Knowles at the 17th International Congress of Theoretical and Applied Mechanics, Grenoble.

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