**"NONLINEAR, DISTORTIVE PHENOMENA IN SOLIDS:
MARTENSITIC, CRACK, AND MULTISCALE STRUCTURES"**

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Progress: 1991-92

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Background: This ongoing program, from the beginning of the first three year grant 1988-1991 and now in the first year of the second phase 1991-1994, has been directed at developing both an understanding of the physics underlying structural transformations in real (alloy) materials as well as new theoretical methods which adequately describe the large (nonlinear) distortions which characterize such processes. We have had a particular interest in martensitic systems, first (1988-1991) in the equilibrium limits, and now (below) in phenomena associated with the transformation process. Both ongoing projects and new projects are progressing vigorously. Moreover, the new collaborative research with co-principal investigators, J.P. Sethna and J.A. Krumhansl, is proving exceedingly productive.

Research Progress

1. First Principles Models of First Order Transformations: (J.A. Morris and R.J. Gooding; W.C. Kerr, A.M. Hawthorne, R.J. Gooding, A.R. Bishop and J.A. Krumhansl). This project, begun in 1989, has come to maturity, with three publications to date. The starting point is a (nonlinear) dynamical model meant to simulate the atomic dynamics of a first order structural transformation. The properties are determined by molecular dynamics and rigorous statistical mechanics. This is believed to be the first fundamental, exact simulation of a structural first order transformation to reproduce the thermodynamic and dynamic behavior of materials like martensites. A major and important issue of principle has been verified: heterophase fluctuations become vanishingly improbable in pure, equilibrium systems. Although that in itself is expected, what has been developed along the way is an understanding of how compositional disorder in real alloys, or defects, may so strongly affect the approach to equilibrium. An example in shape memory alloys is discussed in the next item.

2. Transitional Structures in Shape Memory Alloys: (S. Kartha, T. Castan, J.A. Krumhansl, J.P. Sethna) For many years experimental studies of martensitic transformations in shape memory alloys have found evidence for pretransitional structures. Although certainly some of these are locally transformed regions around special symmetry defects, it

has been found that there is a ubiquitous, common distortive pattern, resembling "tweed," of interlaced partially transformed regions of the variants in the martensitic "phase to be" even though one may be 100-200 K above the transition. Alloy Examples: $\text{Fe}_x\text{PD}_{1-x}$, $\text{Ni}_{.63}\text{Al}_{.37}$, $\text{Ti}_{.50}\text{Ni}_{.50-x}\text{Fe}_x$; High T_c : $\text{YBa}_2(\text{Cu}_{1-x}\text{Co}_x)\text{O}_{7-\delta}$. Were this remarkable structure indeed generic it would have significant consequences in the transformation process. We believe that in fact tweed is real, does not occur in pure defect free material, but can be promoted by almost any (even mild) distribution of deviations from perfect order. We have made a significant breakthrough with a new theoretical model that produces "tweed" in a natural manner in a binary alloy, taking account only the statistical compositional variations. this has been done by adapting the theory of "spin glass" phases to structural transformations for the first time comparisons with experiments are being made.

3. A General Crack Propagation Law: (J. Hodgdon and J.P. Sethna) Also new this year is the development of a principle for crack propagation in fracture, using general ideas borrowed from physics - symmetry, gauge invariance, and gradient expansions. The "principle of local symmetry," used extensively to describe 2-dimensional crack propagation follows automatically, but this new law goes beyond to 3-d cracking. New materials properties then need to be known to describe cracks.

Proposed Research 1992-1993

1. First Principles Studies: The research in this area discussed above was done on pure systems. Both the molecular dynamics and statistical mechanics utilizing the transfer matrix approach can be now extended to disordered systems, or to include defects. Clearly this is next on the agenda.

2. Transitional Structures in First Order Displacive Transformations:

- a. In point of fact the application of the "spin-glass" methods to understand tweed structure in real alloys or high T_c materials has so far only been simulated with clear results for 2-d transformations. This may be relevant to the structural

transitions in some high T_c materials which transform tetragonal to orthorhombic (i.e. square to rectangular in the basal plane, but much smaller changes in the "c" axis). Much data is available and tweed is well verified experimentally in several high T_c systems. We will see how well the theory and experiment agree.

- b. Many of the shape memory alloys, however, are cubic to tetragonal or close packed structures, with at least three allowable product variants. In 3-d it is far more difficult to envisage tweed; indeed perhaps it is more realistic to think of sponge like interpenetrating variants as the generalization of tweed. We've just begun to cope seriously with the 3-d problem; it is tough but there appear to be several possible approaches suggested by the extensive spin-glass literature to exploit.
- c. Assuming that there now is substantial experimental and theoretical evidence for tweed or analogous pretransitional structures, for significant temperature ranges above the actual bulk transformation temperature, there are a large number of "strange" observations for which an explanation may be finally at hand. For example; (i) Softening of ultrasonic measured moduli for many degrees away from transformation, but no softening when measured by neutrons, (ii) Reversible, possible scaling governed, behavior in some plastic flow experiments, where irreversible chaotic dynamics are expected, (iii) The nonlinear magnetic susceptibility of some spin-glasses show singular behavior of critical temperature - does the nonlinear elastic modulus show analogous behavior at the onset of tweed? Quite aside from our theoretical program there are a number of experimentalists with whom we are interacting.

3. Effect of Disorder on Crack Growth: Just as the introduction of disorder into the structural transformation theory has resulted in some highly interesting proposals for transformation precursors, we expect (but can't prove yet) that disorder may well influence crack formation in some important way - at least in some materials. We'll find out.

Publications:

"Exactly Solvable Heterophases Fluctuations at a Vibrational-Entropy-Driven First-

Order Transition," J.R. Morris and R.J. Gooding, Phys. Rev. Lett 65, 1769 (1990).

"Vibrational Entropy Effects at Diffusionless First-Order Solid-to-Solid Transitions," J.R. Morris and R.J. Gooding, Phys. Rev B43, 6057 (1991).

"First-Order Displacive Structural Phase Transitions Studied by Computer Simulation," W.C. Kerr, A.M. Hawthorne, R.J. Gooding, A.R. Bishop, J.A. Krumhansl, Phys. Rev B, in press (1992).

"Finite Size Scaling Study of a First-Order Temperature-Driven Symmetry-Breaking Structural Phase Transition," J.R. Morris and R.J. Gooding, J. Statistical Phys., in press (1992).

"Nonlinear Physics in Martensitic Transformations," J.A. Krumhansl and G.R. Barsch in Martensite, ed. G.B. Olson, American Society of Metals, in press (1992).

"Spin-Glass Nature of Tweed Precursors in Martensite Transformations," S. Kartha, T. Castan, J.A. Krumhansl and J.P. Sethna, Phys. Rev. Lett 67, 3630 (1991).

"*Beyond the Principle of Local Symmetry*: Derivation of a General Crack Propagation Law," J. Hodgdon and J.P. Sethna, submitted to Int. Jour. Structures and Solids (1992).

"Tweed in Martensites: A Potential New Spin Glass," J.P. Sethna, S. Kartha, T. Castan and J.A. Krumhansl, Nobel Symposium, 1991, in press Physica Scripta.

Invited Talks:

J.A. Krumhansl:

"Physics of Martensite," Los Alamos Workshop, Feb. 1991.

"Physics of Martensite," U.S.-Japan Workshop, Brookhaven National Lab, March 1991.

"Nonlinear Physics in Martensite," Northwestern, June 1991.

"Physics of Structural Transformation," Gordon Conferences on Ceramics, Aug. 1991.

"Physics of Shape Memory Alloy," Materials Research Society, Boston, Dec. 1991.

"Mesosstructure: A New Fundamental State of Matter," University of Massachusetts, Dec. 1991.

J.P. Sethna:

"Tweed in Martensite," Los Alamos Workshop, Feb. 1991.

"Tweed in Martensite, " U.S.-Japan Workshop, Brookhaven National Laboratory, March, 1991.

"Tweed in Martensite," NORDITA, September, 1991.

"The Spin-Glass Nature of Tweed in Martensites," Swedish Physical Society, Stockholm, December, 1991.

"The Spin-Glass Nature of Tweed in Martensites," Nobel Symposium, Gothenburg, Sweden, December, 1991.

"The Spin-Glass Nature of Tweed in Martensites," Universitat de Barcelona, Spain, December, 1991.

"The Spin-Glass Nature of Tweed in Martensites," Institute Laue-Langevin, Grenoble, France, Dec. 1991.

Jennifer Hodgdon:

"Crack Growth Laws from Symmetry," NORDITA, September, 1991.

Personnel:

James A. Krumhansl, Professor Emeritus, Cornell

James P. Sethna, Associate Professor, Cornell

James R. Morris, Graduate Student, Cornell (Ph.D. expected, September 1992)

Sivan Kartha, Graduate Student, Cornell (Ph.D. expected, September, 1993)

Jennifer Hodgdon, Graduate Student, Cornell (Ph.D. expected, September, 1992)

Teresa Castan, Visiting Scientist, Associate Professor, University of Barcelona

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