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13. ABSTRACT (*Maximum 200 words*)

James and Kinderlehrer have given a new theory of magnetostriction. The theory shows excellent agreement with experiment and has motivated new experiments on the relation between domain structure and behavior by Lord and by DeGraef. The theory implies a new mechanism for magnetostriction in $Tb_xDy_{1-x}Fe_2$ (x near 0.3). It also strongly suggests the existence of materials (termed "magnetomemory" materials by the authors) that would have magnetostrictive strain that is two orders of magnitude larger than the largest produced by current giant magnetostrictive materials.

Luskin and his research group have developed an advanced computational model for the dynamics of crystals which undergo a martensitic transformation. They have used this model to compute the development of martensitic microstructure and the propagation of the interface separating the austenitic phase from the martensitic phase, and they have obtained results for the influence of the surface energy and the viscosity on the dynamics.

James, Kinderlehrer, Luskin and their collaborators have studied new mechanisms for hysteresis, and have clarified the role of elastic incompatibility, shuffling, kinetics, and microstructure.

14. SUBJECT TERMS magnetostriction, microstructure, shape memory materials, laminates, finite element methods, martensite, weak convergence methods, relaxation, calculus of variations, continuum mechanics, local minima, kinetics, shuffling

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Transitions, Defects, and Whiskered Microstructures

Principal Investigators: Richard James, David Kinderlehrer, Mitchell Luskin

RESEARCH REPORT

James and Kinderlehrer gave a new theory of magnetostriction and have investigated the microstructure and behavior of the highly magnetostrictive material $TbDyFe_2$ (terfenol). One of the main conclusions of this work is that the growth twins in this material do not inhibit the magnetostriction, as was thought by most workers in this field. Further improvements in the material will be limited with regard to the maximum achievable magnetostrictive strain. We propose that to achieve maximum magnetostriction, the material exchanges coarse domains for fine ones. The coarse domains exhibit an exactly coherent structure while the fine phase domain arrangement is only coherent in an average sense. We still think (as described in our proposal) that the best hope for materials with much larger magnetostriction is by combining the shape-memory and magnetostrictive effects. We are currently studying what desirable features an energy function for such a material should have, and we have come up with several possibilities.

Our theory of martensitic transformations continues to have additional applications. A wide variety of microstructures, including simple and complex twin crossings, layers within layers, laminate patches, and wedge-like microstructures observed in CuAlNi are accurately predicted by the theory.

James and Müller continued work on the passage from molecular to continuum theory for magnetism. We think that this type of calculation — the direct derivation of continuum theory from atomic theory — is very promising. These calculations are similar to our microstructure calculations in that weak convergence methods play an important role, except that it is the molecular fields that undergo rapid oscillation. We think that it should be possible to derive new continuum theories in this way.

Ball and James continued research on metastability and hysteresis. The goal is to predict the size of the hysteresis loops observed by C. Chu in his biaxial loading experiments on martensitic Cu-Al-Ni single crystals. His observations on the role of imposed disturbances suggest to us an approach based on calculating the relative minimizers of free energy; these calculations allow large disturbances of the deformation gradient but small disturbances of the deformations. The key idea is that, for reasons of geometric compatibility, a small nucleus of the energetically preferred phase necessarily must be surrounded by a transition layer. The energy penalty for this layer is more than the energy gained due to the presence of the small nucleus. This leads to metastability. The comparison with experiment is good so far.

Kinderlehrer and Ma have studied the computation of magnetostrictive configurations. They are able to produce hysteresis loops for the linear magnetostrictive material, and now have an understanding of the origins of hysteresis in these materials. The basic mechanism is local stability, as discussed above, but not related to geometric compatibility. The computed hysteresis loop does not collapse as the rate of change of the applied field goes to zero. The stability criterion which they have derived from this idea provides a good estimate of the critical field where the system enters an unstable regime analogous to the known Stoner-Wohlfarth condition. This analysis is based on replacing the entire computational system with a simple finite dimensional system intended to mimic the behavior of the closure domains observed in the computation. The major feature is an appropriate discretization of the demagnetization energy. This energy plays an important role in the behavior of large magnetic bodies, like Terfenol actuators. Also underway is the computation of a linear elastic two-dimensional model for the behavior of a twinned dendritic microstructure.

Relaxation of non-convex energy functionals remains a high priority in understanding the actual configurations attained by a material system. Often, in addition to deformation, other quantities appear in the energy. Recently, together with Fonseca and Pedregal, Kinderlehrer has attacked this issue. Beginning from the theory developed with Pedregal about weakly convergent minimizing sequences, it was shown possible to introduce minimizing sequences which both preserve (convex) constraints and integrability. In a companion paper, they treat the case of bounded variation.

Luskin and his research group have developed computational methods which now enable the theory to be used to predict the response of martensitic crystals with microstructure to a much wider class of boundary loads and temperature variations than those accessible to analytic techniques. Our computational program has motivated the development of theory which can give quantitative predictions about experiments. One successful example of this synergy was our development of the energy density for an indium-thallium alloy which we used in our three-dimensional computations of equilibria and dynamics for this crystal with general boundary loads and temperatures (Collins and Luskin [1993], Klouček and Luskin [1994a, 1994b]).

Since the computed deformation gradient approximating the deformation gradient of a solution with microstructure cannot be expected to converge pointwise under mesh refinement, we introduced a theory for the numerical analysis of microstructure which we used to rigorously analyze the convergence of the finite element approximation of several model problems. We showed that an approximate Young measure (which measures the oscillatory behavior of the computed deformation gradient) converges to the Young measure of the solution, and we also proved the convergence of the macroscopic variables defined by the integral of nonlinear functions of the approximate deformation gradients. Our theory for the analysis of numerical methods for microstructure has also allowed us to develop practical guidelines for the development of effective and efficient computational methods (Collins, Luskin, and Riordan [1993], Klouček, Li, and Luskin [1994]).

Luskin and his research group have developed methods and a code to investigate dynamical phenomena associated with martensitic transformations modeled by the balance of linear momentum

$$\rho y_{tt} = \nabla \cdot \sigma, \qquad (x,t) \in \Omega \times (0,\infty), \tag{1}$$

where ρ is the density, $\sigma(\nabla y(x,t), \theta(x,t))$ is the total stress tensor, and the temperature $\theta(x,t)$ is given. Since in our theory

$$\sigma(F,\theta) = \frac{\partial W(F,\theta)}{\partial F} + \text{surface stress} + \text{viscous stress}$$

where $W(F,\theta)$ is the Helmholtz free energy density, the multi-well structure of the Helmholtz free energy density leads to an ill-posed problem (in the absence of surface stress and viscous stress) for the linearized momentum equation about some strains. We have developed stable time-discretization methods and efficient techniques for the solution of the linear equations at each time step even though the energy density if non-convex (Klouček and Luskin [1994b]).

Our computational experiments have simulated the development of martensitic microstructure and the propagation of the austenitic-martensitic phase boundary which separates the homogeneous austenitic phase from the microstructured martensitic phase (Klouček and Luskin [1994a, 1994b]). We have also done computational studies of the effects of surface stress and viscous stress on the dynamics (Klouček and Luskin [1994b]). We have recently developed methods and an extension of our code which includes thermal effects by solving (1) with the equations for the balance of energy

$$\rho e_t = \sigma \cdot \nabla y_t - \nabla \cdot q, \tag{2}$$

for the deformation and temperature where $e(\nabla y(x,t), \theta(x,t))$ is the internal energy density and $q(\nabla y(x,t), \theta(x,t), \nabla\theta(x,t))$ is the heat flux.

We used our theory of numerical analysis for microstructure to give a rigorous analysis of the convergence of a finite element approximation of the magnetization for a ferromagnetic crystal (Luskin and Ma [1992]), and we have developed an extension of the simulated annealing algorithm to solve the numerical optimization problem (Luskin and Ma [1993]). These techniques are being extended to magnetostriction problems (Kinderlehrer and Ma [1994]).

Recently, Abeyaratne, Chu and James have investigated the influence of microstructure on kinetics. The presence of microstructure introduces many little wiggles on the macroscopic energy. They consider gradient-flow kinetics of such energies, which they analyze by a change of scale calculation. The resulting macroscopic kinetic law is completely different from the microscopic one; it shows remarkably good agreement with the dynamic observations of Chu under a wide variety of imposed loading programs.

Bhattacharya, James and Swart [1994] have given a new theory of shuffling and have discussed its implications for hysteresis in shape memory materials that exhibit this phenomenon.

Our theories and computational results are being studied intensely in the mathematical community, and are gaining acceptance by materials scientists. In certain cases they have made definite predictions which have preceded the corresponding experiment; these predictions have subsequently shown excellent agreement with experiment (Chu [1993], James and Kinderlehrer [1994], Bhattacharya, James and Swart [1994]). In other cases the theories have been used to design entirely new experiments (Ball and James [1992], Chu, James and Miyazaki [1994]). These experiments have especially revealed the three dimensional behavior of transforming materials. These tests have also given a wide range of new observations, especially relating to hysteresis.

FINAL TECHNICAL REPORT
AFOSR-91-0301-A
Transitions, Defects, and Whiskered Microstructures
Principal Investigators: Richard James, David Kinderlehrer, Mitchell Luskin

PUBLICATIONS

1. R. Abeyaratne, C. Chu and R. D. James, Kinetics and hysteresis in martensitic single crystals, Proc. Symposium on the Mechanics of Phase Transformations and Shape Memory Alloys, ASME, 1994

2. J. M. Ball C. Chu, and R. D. James, Metastability of martensite, preprint.

3. J. M. Ball and R. D. James, Proposed experimental tests of a theory of fine microstructure and the two well problem. Phil. Trans Royal Soc. Lond. A 338 (1992), 389-450.

4. J. M. Ball and R. D. James, Theory of the microstructure of martensite and applications, Proc. International Conference on Martensitic Transformations, Monterey, 1992, pp. 65-76.

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9. C. Chu and R. D. James, Biaxial loading experiments on martensite single crystals, Proc. ASME conference on Experiments in Smart Materials, 1993.

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17. R. D. James and D. Kinderlehrer, Twinned structures in Terfenol, Proc. International Conference on Martensitic Transformations, Monterey, 1992. R. D. James and D. Kinderlehrer, Theory of magnetostriction with applications to TbDyFe2, Phil. Mag. B, 68, 237-274.

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21. R. D. James and S. Müller, Internal variables and fine scale oscillations in micromagnetics, Continuum Mechanics and Thermodynamics 6 (1994), pp. 291-336.

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24. D. Kinderlehrer, Second variation of liquid crystal energy at $x/|x|$ (with B. Ou), Proceedings Royal Society London (to appear).

25. D. Kinderlehrer, Remarks about surface energy (with G. Vergara Caffarelli), to appear.

26. D. Kinderlehrer, Some methods of analysis in the study of microstructure, Proc. Tenth Army Conf. Appl. Math. and Computing,(1993) 613-631.

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40. N. Simha and L. Truskinovsky, Shear induced transformation toughening in ceramics, Acta. Metallurgia et Materialia 42 (1994), pp. 3827 - 3836.

41. N. Simha, Do habit planes exist for the tetragonal to monoclinic transition in zirconia?, preprint.

42. L. Truskinovsky and G. Zanzotto, Ericksen's bar revisited: finite-scale microstructures and metastability in one-dimensional elasticity, preprint.

ANNUAL TECHNICAL REPORT
AFOSR-91-0301-A

Transitions, Defects, and Whiskered Microstructures

Principal Investigators: Richard James, David Kinderlehrer, Mitchell Luskin

INVITED LECTURES OF RICHARD JAMES

Workshop on Homogenization, Mathematical Sciences Research Institute, 1991
American Association for the Advancement of Science, Washington D. C., 1991
Contemporary Developments in Solid Mechanics, in honor of the 60th birthday of J. K. Knowles, Caltech, 1991
Department of Aerospace Engineering and Mechanics, University of Texas at Austin (colloquium), 1991
Seminar on Dynamics and Flow Systems, University of Minnesota, 1991
Theory of Martensite, a workshop organized by G. Olson, Northwestern, 1991
Army Conference on Applied Mathematics and Computing, University of Minnesota, 1991
The Mathematics of Nonlinear Systems, University of Bath
International Centre for Mathematical Sciences opening meeting on Mathematics in Materials Science, 1991
Workshop on Whiskered Microstructures, Carnegie Mellon University, 1991 (co-organized with D. Kinderlehrer and T. Einstein)
Materials Research Society Meeting on Theory and Applications of Shape-Memory Materials, Boston, 1991
Seminar on Mathematics in Materials Science, Heriot-Watt University, 1991
Applied Mathematics Seminar, Courant Institute, 1991
Department of Mathematics, Carnegie Mellon University, 1991
Edinburgh Mathematics Society and The Royal Society of Edinburgh joint meeting, (lecture to a general audience on paper folding and the microstructure of crystals) 1992
Thermodynamics of Materials, Oberwolfach, 1992
Institut fur Angewandte Mathematik, Universitat Bonn, 1992
School of Mathematics, University of Bath, 1992
Department of Applied Mathematics, University of East Anglia (colloquium), 1992
Department of Mathematics, Sussex University (colloquium), 1992
Department of Applied Mathematics, University of Edinburgh (colloquium), 1992
Transitions de Phase, University of Metz, 1992
Edinburgh International Science Festival (general lecture on "Smart Materials"), 1992
Mathematics in the 21st Century, a panel discussion at the Edinburgh Science Festival (panel member, together with Sir John Kingman(chair), T. B. Benjamin, Feng Kang and Jacob Palais), 1992
The Microstructure of Crystals, conference at the ICMS co-organized with J. M. Ball, 1992
Micromagnetics and Magnetostriction, conference at the ICMS co-organized with D. G. Lord and A. De Simone), 1992
Science Now, BBC Radio 4 (popular talk on "Smart Materials"), 1992
BBC World Service (popular talk on "Smart Materials"), 1992
International Conference on Martensitic Transformations, Monterey, 1992
Workshop on Computational Methods in Materials Science (Organizer, with R. A. Nicolaides, D. Kinderlehrer and J. Turner), Carnegie-Mellon University, 1992
Society for Natural Philosophy, Pennsylvania State University, 1992
Department of Mathematics, Worcester Polytechnic Institute (colloquium), 1992
Center for the Mechanics of Composites, Texas A&M University (colloquium), 1992
Society of Photo-Optical Instrumentation Engineers conference on Smart Structures and Materials, 1993
Eleventh Army Conference on Applied Mathematics and Computing, Carnegie-Mellon University, 1993
Workshop on Metastability and Hysteresis, International Centre for Mathematical Sciences, Edinburgh, 1993
Phase Transitions, informal meeting at Talbot House, South Pomfret, Vermont, 1993
Society of Photo-Optical Instrumentation Engineers conference on Smart Structures and Materials, 1993
Eleventh Army Conference on Applied Mathematics and Computing, Carnegie-Mellon University, 1993
Workshop on Metastability and Hysteresis, International Centre for Mathematical Sciences, Edinburgh, 1993
Phase Transitions, informal meeting at Talbot House, South Pomfret, Vermont, 1993

A gathering of research workers with interests on the metastability, hysteresis, kinetics and microstructure of martensite, University of Minnesota, (host), 1993
Department of Mechanical Engineering, M.I.T. (colloquium), 1993
International Centre for Mechanical Sciences, Udine (8 lectures on Shape-Memory Materials), 1993
Magnetics group, Metals Development, Ames Lab, Iowa State University, 1993
Institute for Advanced Study, Princeton, PDE seminar, 1993
Department of Theoretical and Applied Mechanics, University of Illinois, Champaign-Urbana (colloquium), 1993
Workshop on Material Microstructure, Institute for Advanced Study, Princeton, 1993
Seminar on Materials Science, Courant Institute of Mathematical Sciences, 1994
Workshop on Micromechanics of Small Volumes, Institute for Mechanics and Materials, San Diego (lecture and co-organizer), 1994
SPIE Conference on Smart Structures and Materials (lecture and program committee), 1994
SIAM Conference on Emerging Issues in Mathematics and Computation from the Materials Sciences, Pittsburgh (principal lecture), 1994
National Institute of Standards and Technology, Gaithersburg (seminar), 1994
Department of Mechanical Engineering, Johns Hopkins University (colloquium), 1994
12th US National Congress on Applied Mechanics, Seattle, 1994
Meeting on Calculus of Variations and Discontinuous Structures, Como, Italy (lecture), 1994
38th meeting of the Society for Natural Philosophy, Cornell University, Ithaca (lecture), 1994
31st Meeting of the Society for Engineering Science, Texas A & M University, College Station (presentations), 1994
Adaptive Quiet Structures with Active Materials, University of Maryland (Research summary), 1994
ASME Symposium on the Mechanics of Phase Transformations and Shape Memory Alloys, Chicago (presentation), 1994
Applied Mechanics, Division of Applied Sciences, CalTech (colloquium), 1994
Mathematical Problems in Micromagnetics, Freiburg, Germany (lecture and colloquium), 1994
DMV-Seminar 1994, Lecture series on "The Mathematics of Microstructure" organized by the German Mathematical Society, Heinrich-Fabri Institut, Blaubeuren (10 lectures with J. M. Ball), 1994

RECENT INVITED LECTURES OF DAVID KINDERLEHRER

First European conference on elliptic and parabolic problems, Pont a Mousson, 1991
Mathematical Sciences Research Institute, 1991
Three Rivers Applied Mathematics Colloquium, 1991
American Association for the Advancement of Science Symposium, 1991
ICIAM Conference, 1991
Rice University, 1991
University of Houston, 1991
Pont a Mousson, France June 17 First European Conference on Elliptic and Parabolic Problems
Paris, France June 20 Coll ge de France
Washington, DC July 12 International Conference on Industrial and Applied Mathematics
CMU, Pittsburgh, PA Sept. 27 Inaugural Conference of the Center for Nonlinear Analysis
Leesburg, VA Oct. 18 SIAM Conference on Mathematical Methods in Material Microstructure
Hampton University Nov. 16 Center for Nonlinear Analysis Research Workshop
University of Indiana Dec. 5 Colloquium, Dept. of Mathematics
Case Western Reserve Jan. 30 Joint Colloquium, Depts of Chemical Engineering and Mathematics
Kent State University March 6 Joint Colloquium, Liquid Crystal Institute and Dept. of Mathematics
Pennsylvania State U. March 16 Applied Mathematics Seminar
Rome, Italy April 8 Seminar, Istituto per le Applicazioni del Calcolo
Rome, Italy April 10 Seminar, Istituto per le Applicazioni del Calco lo
Edinburgh, Scotland June International Centre for Mathematical Sciences programme on Mathematical Problems in M aterials Science
West Point, NY June 18 Tenth Army Conference on Applied Mathematics and

Computing
Monterey, CA July 21 ICOMAT-92
Kent State University, 1992, ALCOM/IMA conference on Computational Problems in Liquid Crystals
Albequerque, NM, 1993, SPIE Smart Structures and Materials 93
Paris, 1993, College de France
Metz, 1993, Metz Days
New York, 1993, Courant Institute
Brown, Providence, 1993
Athens, Ohio, 1993
Trieste, Italy, 1993
Metz Days, Univ. de Metz, 1993
Conference on Differential Equations, Athens, OH, 1993
Joint TMS/ASM meeting, Pittsburgh, 1993
Mathematical Methods for Microstructure, Institute for Advanced Study, Princeton, 1993
SISSA conference: Homogenization and related topics,Trieste, Italy, 1993
Spring Lecture Series (Principal lecturer), University of Arkansas, 1994
SIAM Meeting on emerging Issues in Mathematics and Computation from the Materials Sciences, conference chair, 1994
Conference on Industrial and Applied Mathematics, Linkoping, Sweden, 1994
Mechanical and Analytical Microstructures, Accademia dei Lincei, Rome, 1994
SPIE Smart Structures and Materials 94, Orlando, FL
Joint MMM/Intermag meeting, Albuquerque, NM, 1994
Solid/Solid Phase Transitions in Inorganic Materials 94 (TMS), Nemacolin Woods, PA, 1994
Society of Engineering Science, 1994
Variational methods for discontinuous structures, Como, Italy, 1994
College de France, Paris, 1993
Courant Institute, New York, 1993
Brown University, Providence, 1993
University of Minnesota (Dept. of Aerospace Engineering and Mechanics), 1993
IAC, Rome, Italy, 1993
Colloquium, Department of Materials Science and Engineering, CMU, 1994
Scientific Presentation, ARO Annual Review, Research Triangle Park, 1994
Institute for Advanced Study, Princeton, 1994

RECENT INVITED LECTURES OF MITCHELL LUSKIN

Imperial College, London, July 12, 1991
Euromech Colloquium 283, University of Strathclyde, Glasgow, July 18, 1991
13th IMACS World Congress on Computation and Applied Mathematics, Trinity College, Dublin, July 22, 1991
IMA, Minneapolis, Tutorial Workshop for Special Year on Applied Linear Algebra, September 4, 1991
Xi'an Jiaotong University, China, October 21, 1991
Peking University, Department of Mechanics, October 24, 1991
Academia Sinica, Applied Mathematics, October 25, 1991
Peking University, Department of Mathematics, October 26, 1991
Tsinghua University, October 26, 1991
Academia Sinica, Systems Science, October 27, 1991
Ryukoku University, Otsu, Japan, October 29, 1991
Kyoto University, Research Institute for Mathematical Sciences, October 30, 1991
Penn State University, Math Colloquium, November 22, 1992
Materials Research Society Annual Meeting, Boston, December 3, 1991
Rice University, January 29, 1992
University of Houston, January 31, 1992
Brown University, April 9, 1992
University of Chicago, May 1, 1992

University of Maryland, May 7, 1992
International Centre for Mathematical Sciences, Edinburgh, June 9, 1992
International Centre for Mathematical Sciences, Edinburgh, June 16, 1992
International Conference on Martensitic Transformations, Monterey, July 20, 1992
Center for Nonlinear Analysis, Carnegie Mellon University, September 16, 1992
Society for Natural Philosophy, Penn State University, October 3, 1992
Liquid Crystal Institute, Kent State University, November 13, 1992
Oberwolfach Mathematics Institute, Germany, December 7, 1992
University of Warsaw, December 11, 1992 and December 14, 1992
Academy of Science of the Czech Republic, Institute of Computing Sciences, Prague, December 17, 1992
Society of Photo-Optical Instrumentation Engineers Conference on Smart Structures and Materials, Albuquerque, February 3, 1993
University of New Mexico, February 3, 1993
American Association for the Advancement of Science Annual Meeting, Boston, February 16, 1993
AFOSR Meeting on Computational Mathematics, Washington University, St. Louis, May 20, 1993
Institute for Advanced Studies in Mathematics, Technion, Israel, Workshop on Defects in Nonlinear Media, June 14, 1993
International Colloquium on Free Boundary Problems, Toledo, Spain, June 22, 1993
Progress in the Theory and Application of the Finite Element Method II, Chalmers University of Technology, Gothenburg, Sweden, August 28, 1993
Center for Nonlinear Partial Differential Equations, Delft Institute of Technology, Delft, Netherlands, August 31, 1993
The Finite Element Method: Fifty Years of the Courant Element, University of Jyväskylä, Jyväskylä, Finland, September 2, 1993
Courant Institute, New York University, New York, December 2, 1993
Institute for Advanced Study, Princeton, New Jersey, December 6, 1993
University of California, Los Angeles, January 3, 1994
SIAM Conference on Emerging Issues in Mathematics and Computation from the Materials Sciences, Pittsburgh, Pennsylvania, April 18, 1994
Massachusetts Institute of Technology, Department of Mechanical Engineering April, 28, 1994
Brown University, Department of Applied Mathematics April 29, 1994
European Conference on Elliptic and Parabolic Problems, Pont-à-Mousson, France, June 13, 1994
University of Crete, Greece June 21, 1994