EVOLUTION OF PHASE TRANSITIONS

This work began with the authors' exploration of the applicability of the finite deformation theory of elasticity when various standard assumptions such as convexity of the energy or ellipticity of the field equations of equilibrium are relinquished. The finite deformation theory of elasticity turns out to be a natural vehicle for the study of phase transitions in solids where thermal effects can be neglected. This is a valuable work for those interested in the development and application of continuum-mechanical models that describe the macroscopic response of materials capable of undergoing stress- or temperature-induced transitions, which may be either dynamic or quasi-static, controlled by a kinetic relation that in the framework of classical thermomechanics represents information that is supplementary to the usual balance principles and constitutive laws of conventional theory. The book should be of interest to mechanicians, material scientists, geophysicists, and applied mathematicians.

Rohan Abeyaratne is the Quentin Berg Professor of Mechanics and Head of the Department of Mechanical Engineering at MIT. He received his bachelor's degree from the University of Ceylon and his doctorate from the California Institute of Technology. Among his honors are the E.O.E. Pereira Gold Medal (1975), Den Hartog Distinguished Educator (1995), MacVicar Fellowship (2000), Fellow, American Academy of Mechanics (1996) and Fellow, American Society of Mechanical Engineers (1998). His primary research interest is in nonlinear phenomena in mechanics.

James K. Knowles is the William R. Kenan Professor of Applied Mechanics, Emeritus, at the California Institute of Technology. He received his S.B. and Ph.D. degrees from MIT, and he holds an honorary Sc.D. degree from the National University of Ireland. He is a Fellow of the American Academy of Mechanics (AAM), the American Association for the Advancement of Science and the American Society of Mechanical Engineers (ASME). He is a past president of AAM, and he is a recipient of MIT's Goodwin Medal for teaching, the Eringen Medal of the Society of Engineering Science and the Koiter Medal of the ASME. His primary research interests are in nonlinear phenomena in continuum mechanics, and in analytical issues in fracture mechanics and the theory of elasticity.

EVOLUTION OF PHASE TRANSITIONS

A Continuum Theory

ROHAN ABEYARATNE

Massachusetts Institute of Technology

JAMES K. KNOWLES

California Institute of Technology



> CAMBRIDGE UNIVERSITY PRESS Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo

Cambridge University Press 40 West 20th Street, New York, NY 10011-4211, USA

www.cambridge.org Information on this title: www.cambridge.org/9780521661478

© Cambridge University Press 2006

This publication is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First published 2006

Printed in the United States of America

A catalog record for this publication is available from the British Library.

Library of Congress Cataloging in Publication Data

Abeyaratne, Rohan.
Evolution of phase transitions : a continuum theory / Rohan Abeyaratne, James K. Knowles. p. cm.
Includes bibliographical references and index.
ISBN-13: 978-0-521-66147-8
ISBN-10: 0-521-66147-1
Phase transformations (Statistical physics). 2. Continuum mechanics.
Kinetic theory of matter. I. Knowles, James K. (James Kenyon), 1931– II. Title
QC175.16.P5A24 2006
530.4'74—dc22 2005033285

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for external or third-party Internet Web sites referred to in this publication and does not guarantee that any content on such Web sites is, or will remain, accurate or appropriate.

To the C7: Gina, Kenny, Kevin, Kristen, Liam, Linus, & Nina;

and the J4: Jackie, John, Jeff, & Jamey.

Contents

Pr	eface	e page	xiii
]	Part	I Introduction	
1	Intr	oduction	3
	1.1	What this monograph is about	3
	1.2	Some experiments	7
	1.3	Continuum mechanics	9
	1.4	Quasilinear systems	10
	1.5	Outline of monograph	11
P	art I	I Purely Mechanical Theory	
2	Two	-Well Potentials, Governing Equations	
		Energetics	. 19
	2.1	Introduction	19
	2.2	Two-phase nonlinearly elastic materials	20
	2.3	Field equations and jump conditions	25
	2.4	Energetics of motion, driving force and dissipation	
		inequality	27
3	Equ	ilibrium Phase Mixtures and Quasistatic	
	Pro	cesses	. 32
	3.1	Introduction	32
	3.2	Equilibrium states	33
	3.3	Variational theory of equilibrium mixtures	
		of phases	37
	3.4	Quasistatic processes	42
	3.5	Nucleation and kinetics	44
	3.6	Constant elongation rate processes	47
	3.7	Hysteresis	53

CAMBRIDGE

viii

Cambridge University Press
0521661471 - Evolution of Phase Transitions: A Continuum Theory
Rohan Abeyaratne and James K. Knowles
Frontmatter
Moreinformation

CONTENTS	;
----------	---

4	Impact-Induced Transitions in Two-Phase	
	Elastic Materials	. 59
	4.1 Introduction	59
	4.2 The impact problem for trilinear two-phase	
	materials	61
	4.2.1 The constitutive law	61
	4.2.2 The impact problem	64
	4.3 Scale-invariant solutions of the impact problem	66
	4.3.1 Solutions without a phase transition	66
	4.3.2 Solutions with a phase transition: The two-wave case	67
	4.3.3 Solutions with a phase transition: The one-wave case	68
	4.3.4 The totality of solutions	69
	4.4 Nucleation and kinetics	71
	4.5 Comparison with experiment	74
	4.6 Other types of kinetic relations	77
	4.7 Related work	77
Pa	rt III Thermomechanical Theory	
	Multiple-Well Free Energy Potentials	85
5	5.1 Introduction	85
	5.2 Helmholtz free energy potential	86
	5.3 Potential energy function and the effect of stress	88
	5.4 Example 1: The van der Waals Fluid	90
	5.5 Example 2: Two-phase martensitic material	20
	with cubic and tetragonal phases	95
6	The Continuum Theory of Driving Force	105
0	6.1 Introduction	105
	6.2 Balance laws, field equations and jump conditions	105
	6.2.1 Balances of momentum and energy in	100
	integral form	106
	6.2.2 Localization of the balance laws	106
	6.3 The second law of thermodynamics and	100
	the driving force	108
	6.3.1 Entropy production rate	108
	6.3.2 Driving force and the second law	110
	6.3.3 Driving force in the case of mechanical	
	equilibrium	111
7	Thermoelastic Materials	113
/	7.1 Introduction	113
	7.2 The thermoelastic constitutive law	113
	7.2.1 Relations among stress, deformation gradient,	113
	temperature and specific entropy	113
	competature and specific entropy	113

CONTENTS

	7.2.2 The heat conduction law	116
	7.2.3 The partial differential equations of nonlinear	
	thermoelasticity	116
	7.2.4 Thermomechanical equilibrium	117
	7.3 Stability of a thermoelastic material	118
	7.4 A one-dimensional special case: uniaxial strain	120
8	Kinetics and Nucleation	. 124
	8.1 Introduction	124
	8.2 Nonequilibrium processes, thermodynamic fluxes	
	and forces, kinetic relation	124
	8.3 Phenomenological examples of kinetic	
	relations	127
	8.4 Micromechanically based examples	
	of kinetic relations	128
	8.4.1 Viscosity-strain gradient model	130
	8.4.2 Thermal activation model	131
	8.4.3 Propagation through a row of	
	imperfections	133
	8.4.4 Kinetics from atomistic considerations	134
	8.4.5 Frenkel-Kontorowa model	136
	8.5 Nucleation	139
Pa	rt IV One-Dimensional Thermoelastic Theory and Problems	

9	9 Models for Two-Phase Thermoelastic Materials		
	in One Dimension	149	
	9.1 Preliminaries	149	
	9.2 Materials of Mie-Grüneisen type	151	
	9.3 Two-phase Mie-Grüneisen materials	153	
	9.3.1 The trilinear material	153	
	9.3.2 Stability of phases of the trilinear material	156	
	9.3.3 Other two-phase materials of Mie-Grüneisen		
	type	159	
10	Quasistatic Hysteresis in Two-Phase Thermoelastic		
	Tensile Bars	163	
	10.1 Preliminaries	163	
	10.2 Thermomechanical equilibrium states		
	for a two-phase material	164	
	10.3 Quasistatic processes	166	
	10.4 Trilinear thermoelastic material	167	
	10.5 Stress cycles at constant temperature	169	
	10.6 Temperature cycles at constant stress	173	

ix

CAMBRIDGE

Cambridge University Press
0521661471 - Evolution of Phase Transitions: A Continuum Theory
Rohan Abeyaratne and James K. Knowles
Frontmatter
Moreinformation

x		CONTENTS
10.7 The shape-memory cycle	175	
10.8 The experiments of Shaw and Kyriakides	176	
10.9 Slow thermomechanical processes	178	
11 Dynamics of Phase Transitions in Uniaxially Strained		
Thermoelastic Solids	181	
11.1 Introduction	181	
11.2 Uniaxial strain in adiabatic thermoelasticity 11.2.1 Field equations, jump conditions and	182	
driving force 11.2.2 The trilinear Mie-Grüneisen thermoelastic	182	
material	183	
11.3 The impact problem	185	
11.3.1 Formulation: Scale-invariant solutions	185	
11.3.2 Solutions with no phase transition	186	
11.3.3 Solutions with a phase transition	188	
Part V Higher Dimensional Problems		
12 Statics: Geometric Compatibility	197	
12.1 Preliminaries	197	
12.2 Examples	200	
13 Dynamics: Impact-Induced Transition in a CuAlNi		
Single Crystal	209	
13.1 Introduction	209	
13.2 Preliminaries	210	
13.3 Impact without phase transformation	212	
13.4 Impact with phase transformation	214	
13.5 Application to austenite- β'_1 martensite		
transformation in CuAlNi	217	
13.5.1 Experimental data	217	
13.5.2 Phase boundary speed	218	
13.5.3 Driving force	218	
13.5.4 Kinetic law	219	
14 Quasistatics: Kinetics of Martensitic Twinning	221	
14.1 Introduction	221	
14.2 The material and loading device	222	
14.3 Observations	223	
14.4 The model	225	
14.5 The energy of the system	226	
14.5.1 Elastic energy of the specimen	226	
14.5.2 Loading device energy	227	
14.5.3 Summary	228	

CONTENTS

14.6 The effect of the transition layers: Further
observations22914.7 The effect of the transition layers: Further modeling23014.8 Kinetics231Author Index235Subject Index238

Preface

This monograph threads together a series of research studies carried out by the authors over a period of some fifteen years or so. It is concerned with the development and application of continuum-mechanical models that describe the macroscopic response of materials capable of undergoing stress- or temperature-induced transitions between two solid phases.

Roughly speaking, there are two types of physical settings that provide the motivation for this kind of modeling. One is that associated with slow mechanical or thermal loading of alloys such as nickel–titanium or copper–aluminum–nickel that exhibit the shape-memory effect. The second arises from high-speed impact experiments in which metallic or ceramic targets are struck by moving projectiles; the objective of such studies – often of interest in geophysics – is usually to determine the response of the impacted material to very high pressures. Phase transitions are an essential feature of the shape-memory effect, and they frequently occur in highspeed impact experiments on solids. Those aspects of the theory presented here that are purely phenomenological may well have broader relevance, in the sense that they may be applicable to materials that transform between two "states," for example, the ordered and disordered states of a polymer.

Our development focuses on the evolution of the phase transitions modeled here, which may be either dynamic or quasistatic. Such evolution is controlled by a "kinetic relation," which, in the framework of classical thermomechanics, represents information supplementary to the usual balance principles and constitutive laws of conventional theory. We elucidate the rather remarkable way in which the classical theory "calls for" this kind of supplementary information when the material is capable of changing phase, though such additional information is *not* called for – indeed, cannot be imposed – in the case of a single-phase material.

The simplest context in which to illustrate the need for kinetic relations and the role they play is that furnished by the purely mechanical theory of one-dimensional nonlinear elasticity, with thermal effects suppressed. After the Introduction, which comprises Part I of the monograph, we pursue the subject in this context in Part II. Even this simplest version of the theory to be set out here has some utility, as we show in Chapters 3 and 4. Part III presents the full three-dimensional theory, taking

xiii

xiv

PREFACE

both mechanical and thermal effects into account. We specialize this theory to one space dimension in Part IV, where we are able to make some comparisons with experiments. In Part V, we discuss some three-dimensional problems.

The material presented here is drawn primarily from our own research over the period from the late 1980s forward. We came to this subject as practitioners of solid mechanics interested in exploring the range of applicability of the finite deformation theory of elasticity when various standard assumptions such as convexity of various energies or ellipticity of the field equations of equilibrium were relinquished. When broadened in this way, finite elasticity is a natural vehicle for the study of those aspects of phase transitions in solids that can be discussed with thermal effects neglected. Nonlinear *thermoelasticity*, similarly unencumbered by conventional restrictions, provides the natural framework for the study of mechanical and thermal effects together.

Our hope is that this book will be of interest to materials scientists, engineers and geophysicists as well as to mechanicians and applied mathematicians. The perfectly prepared reader would be acquainted with continuum mechanics at the level of Chadwick's *Continuum Mechanics*, Wiley, New York, 1976; with thermodynamics as treated, for example, in J. L. Ericksen's *Introduction to the Thermodynamics of Solids*, Chapman and Hall, New York, 1991; with material behavior as described by T. H. Courtney in *Mechanical Behavior of Materials*, McGraw-Hill, New York, 1990; with partial differential equations at the level of J. D. Logan's *An Introduction to Nonlinear Partial Differential Equations*, Wiley-Interscience, New York, 1994; and with the elements of Cartesian tensors as discussed, for example, in *Linear Vector Spaces and Cartesian Tensors*, Oxford, New York, 1998, by J. K. Knowles. However, expecting many potential readers to be less than perfectly prepared, we have tried to make the presentation as self-contained as is practicable, citing appropriate sources for those results that are used but not derived.

Although the book deals almost entirely with our own work, we have nevertheless had the enormous benefit of interactions with many others, and it is a pleasure to acknowledge them *all* with gratitude. We would be remiss not to mention the particular influence that Tom Ahrens, Kaushik Bhattacharya, Mort Gurtin, Rick James, Stelios Kyriakides, Jim Rice, the late Eli Sternberg, Lev Truskinovsky, and our former doctoral students, especially Phoebus Rosakis and Stewart Silling, have had on our learning of this subject.

Some of the fruitful interactions alluded to above took place in small, informal summer gatherings held at MIT's Talbot House in South Pomfret, Vermont. We are indebted to MIT for the use of this wonderful place, which - alas - is no longer owned by MIT.

Special thanks go to Debbie Blanchard, who drew the figures in the early part of the book, and then taught us how to draw the rest.

We are grateful to Olaf Weckner for a careful and constructive critical reading of the early chapters.

We acknowledge with thanks the past financial support of the U.S. National Science Foundation, the U.S. Army Research Office, and especially the U.S. Office

PREFACE

xv

of Naval Research, with which we enjoyed a sustained relationship and which supported much of the research on which this monograph is based. We would particularly like to thank Roshdy Barsoum, Alan Kushner, and Yapa Rajapakse for the help and encouragement that they, as program officers at ONR, consistently provided to us.

During recent stimulating visits, both of us have benefited from the hospitality and financial support of the University of Cambridge, its colleges, and its Isaac Newton Institute for the Mathematical Sciences, for which we wish to express our appreciation.

> Rohan Abeyaratne and Jim Knowles Cambridge, Massachusetts, and Pasadena, California June 2005