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Solid Mechanics and its Applications

Nonlinear Mechanics of Crystals

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Nonlinear Mechanics of Crystals

SOLID MECHANICS AND ITS APPLICATIONS

Volume 177

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Aims and Scope of the Series

The fundamental questions arising in mechanics are: *Why?*, *How?*, and *How much?* The aim of this series is to provide lucid accounts written by authoritative researchers giving vision and insight in answering these questions on the subject of mechanics as it relates to solids.

The scope of the series covers the entire spectrum of solid mechanics. Thus it includes the foundation of mechanics; variational formulations; computational mechanics; statics, kinematics and dynamics of rigid and elastic bodies: vibrations of solids and structures; dynamical systems and chaos; the theories of elasticity, plasticity and viscoelasticity; composite materials; rods, beams, shells and membranes; structural control and stability; soils, rocks and geomechanics; fracture; tribology; experimental mechanics; biomechanics and machine design.

The median level of presentation is the first year graduate student. Some texts are monographs defining the current state of the field; others are accessible to final year undergraduates; but essentially the emphasis is on readability and clarity.

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Preface

This book presents mathematical descriptions of behavior of crystalline solids following theoretical methods of modern continuum mechanics. Emphasis is placed on geometrically nonlinear descriptions, i.e., finite or large deformations. Topics include elasticity, plasticity, and ways of representing effects of distributions of defects or flaws in the solid on the material's thermomechanical response. Defects may include crystal dislocations, point defects such as vacancies or interstitial atoms, rotational defects, deformation twins, voids or pores, and micro-cracks. Representative substances towards which modeling techniques forwarded here may be applied are single crystalline and polycrystalline metals and alloys, ceramics, minerals, and other geologic materials and their constituents.

An early and substantial part of the text is devoted to kinematics of finite deformations, multiplicative inelasticity, and representations of lattice defects in a differential-geometric setting. An accurate depiction of kinematics is deemed necessary in order to accompany rigorous models of thermodynamics and kinetics of material behavior, since kinematic assumptions tend to enter, implicitly or explicitly, subsequent thermodynamic and kinetic relations. Descriptions and derivations of fundamental mechanical and thermodynamic balance laws and inequalities are then given. Constitutive frameworks are provided for representing thermomechanical behaviors of various classes of crystalline materials: elastic solids, elastic-plastic solids, generalized inelastic solids with lattice defects, and dielectric solids. In each case, material responses corresponding to large deformations are emphasized, though complementary geometrically linear theories are included in some cases for completeness and for comparison with their nonlinear counterparts. General kinetic concepts are described, but relatively less attention is directed towards development of specific kinetic relations, since these tend to be more strongly dependent upon microstructures of particular materials (e.g., crystal structure or chemical composition) within each general class of materials considered. Appendices provide supporting discussion on crystal symmetry and material coefficients, atomistic methods (i.e., lattice statics and origins of stress and elastic coefficients), and elastic models of discrete line and point defects in crystals. The content of this book consists of a combination of the author's interpretation and consolidation of existing science from historic and more recent literature, as well as a number of novel—and sometimes less conventional—theoretical modeling concepts, the latter often presented, developed, or refined by the author (and collaborators in many cases) in a number of archival publications over the past ten years. With a few exceptions, the text is written in the context of generalized (e.g., curvilinear) coordinates, a rarity among other recent texts and monographs dealing with similar subject matter.

This book is intended for use by scientists and engineers involved in advanced constitutive modeling of nonlinear mechanical behavior of crystalline materials. Knowledge of fundamentals of continuum mechanics and tensor calculus is a prerequisite for accessing much of the material in the text. The book could conceivably be used as supplemental material in graduate-level courses in continuum mechanics, elasticity, plasticity, micromechanics, or dislocation mechanics, for students in various disciplines of engineering, materials science, applied mathematics, or condensed matter physics.

A number of individuals have contributed, directly or indirectly, to the content or production of this work; a number have suggested specific changes to early drafts resulting in significant overall improvement to the final manuscript. Technical discussions, interactions, and/or close collaborations with the following individuals over the past decade are gratefully acknowledged (in alphabetical order): Doug Bammann, Peter Chung, Datta Dandekar, Misha Grinfeld, Jarek Knap, Dave McDowell, Rich Regueiro, Mike Scheidler, and Tim Wright. However, any technical inconsistencies, unjust omissions, or errors that may remain are entirely my own. I also appreciate support and resources of the U.S. Army Research Laboratory (formerly known as U.S. Army Ballistics Research Laboratories), including a diligent library staff that was able to efficiently provide or obtain a number of historical works referenced in this text. Finally, I am most appreciative of my wife and daughter, who have remained supportive and patient during the many hours I have spent working on this book over the past 3½ years.

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1 Introduction

1.1 Objectives and Scope

This book presents modeling techniques, primarily from the standpoint of modern continuum mechanics, for describing the nonlinear response of crystalline solids subjected to mechanical loading or deformation. This response may be deformation induced by applied loading, or the forces required to induce such deformation. Nonlinearity may emerge in the geometric sense, pertaining to finite deformations, and/or in the material sense, pertaining to nonlinear relationships among independent and dependent state variables, for example relationships between strain and stress. Though mechanical behavior is of primary interest in this book, thermodynamic principles are exercised for developing descriptions of material behavior also dependent on temperature and internal state variables and consistent with known balance laws or inequalities such as conservation of energy and production of entropy.

Though some physical and mathematical principles applicable towards descriptions of all kinds of materials are supplied in early Chapters, the content of this book is primarily focused on crystalline solids. A crystal refers to a body whose atoms occupy an ordered, repeating structure called a lattice. Defects in the crystal may disrupt the regularity of the lattice, and certain types of point, line, and surface defects are addressed explicitly in this book. A body with defects is still considered here to be crystalline so long as a large percentage of its atoms maintain a repeating, ordered structure. In various instances throughout the text, single- or polycrystalline materials are considered, as are homogeneous and heterogeneous solids. In a single crystal, the lattice is for the most part aligned in a uniform orientation, whereas a polycrystal consists of multiple single crystals or grains aligned in potentially different directions, with constituent crystals separated by grain boundaries. Heterogeneous materials exhibit spatial variations in material properties, for example composites consisting of different phases with different chemical compositions or different crystal

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structures. Specific examples of heterogeneous solids include metal-matrix composites and geologic and cementious materials with several crystalline constituents, e.g., minerals of various crystal structures. In contrast, single crystals are conventionally idealized as homogeneous, at least when their defect content is low. During the course of deformation or a change in environment, initially homogeneous single crystals can become heterogeneous. For example, misoriented subgranular regions can emerge within metallic crystals deformed plastically to large strains.

Detailed consideration of material nonlinearity requires a description of microstructure and defects in the solid, including effects of such defects on kinematics of deformation and on the thermodynamic state of the material. Furthermore, kinetic relations are often required to dictate the temporal evolution of defect distributions and to account for their motions and dissipated energy during time-dependent problems. Defects considered explicitly in this text include distributions of dislocations, rotational line defects, deformation twins, vacancies, and voids.

Chapter 2 provides mathematical background used subsequently throughout the text. Chapter 2 begins with a description of general curvilinear coordinates and related definitions from differential geometry and tensor algebra on manifolds. Such definitions emerge frequently later in presentations of theories of continuously distributed lattice defects. A thorough treatment of the deformation gradient, a fundamental kinematic variable used in continuum mechanical descriptions of constitutive behavior, is provided. This treatment includes discussion of push-forward and pull-back operations, useful identities associated with the deformation gradient, and deformation measures derived from it. Chapter 2 also presents two identities from tensor calculus used often later in the text: Gauss's theorem—a particular version of which is often called the divergence theorem—and Stokes's theorem. Compatibility conditions for finite deformation are discussed, and anholonomic spaces are introduced.

Chapter 3 focuses on descriptions of deformation kinematics of crystalline bodies. This Chapter begins with the fundamental hypothesis of Cauchy and Born describing homogeneous deformations of Bravais lattice vectors and basis vectors comprising the structure of a perfect crystal. Kinematics of multiplicative inelasticity is then considered. The intermediate configuration that emerges under the assumption of multiplicative deformation gradient kinematics is addressed from a general geometric point of view, regardless of the physical origin of inelastic response. Then particular physical sources of non-recoverable deformation are treated in various kinematic descriptions. These include dislocation-based large deformation plasticity of single- and polycrystalline materials, generation and motion of point defects, porosity evolution, and sources of residual elastic deformation of the lattice emerging from multiscale considerations. Chapter 3 then addresses generalized continua embedded with additional kinematic degrees of freedom that describe spatial gradients of deformation of lattice director vectors, whereby locally inhomogeneous deformations can often be associated with the presence of lattice defects. These additional degrees of freedom are introduced in the differential-geometric context of a linear connection on a spatial manifold whose tangent bundle is spanned by a field of deformed director vectors. Geometric properties of the connection enable physical characterization of deformation incompatibilities resulting from continuous distributions of line and point defects.

Chapter 4 features general, traditional thermodynamic relationships and balance laws governing nonlinear behaviors of continuous bodies. The discussion begins with presentation of traditional mass, momentum, and energy balances. Mappings of balance equations among configurations or deformation states are given. Thermodynamic potentials are defined. The internal state variable concept is introduced, enabling representation of effects of defects or evolving microstructure in the description of the thermodynamic state of the material. The dissipation inequality is presented, followed by a brief introduction to kinetic relations and dissipation potentials. Governing equations for generalized continua supporting higher-order stresses (e.g., couple stresses) and those incorporating electromechanical effects are addressed on a case-by-case basis in later Chapters.

Chapter 5 considers elastically deforming solids, a description most applicable to defect-free crystals or to those wherein any effects of defects are not considered explicitly. Constitutive functions and thermodynamic relationships are presented for crystals displaying a hyperelastic response with temperature changes. Thermoelastic material coefficients pertinent to arbitrary three-dimensional stress states, and then those specifically applicable to (but not always limited to) spherical stress states, are defined or derived. Reductions of the general theory of nonlinear anisotropic thermoelasticity under conditions of material linearity, geometric linearity, and isotropic symmetry are described. A thorough presentation of symmetry operations, anisotropy, and material coefficients for all thirty-two crystal classes is provided as supplementary supporting material in Appendix A. An alternative version of finite elasticity with explicitly delineated mechanical and thermal deformations is then developed. Next, Lagrangian field theory of elasticity is presented, wherein governing equations are deduced from Hamilton's principle. Chapter 5 concludes with a discussion of second-grade hyperelasticity, a kind of generalized continuum theory.

Chapter 6 deals with elastoplastic materials. The kinematic description consists of a multiplicative decomposition of the deformation gradient into two terms: the lattice-altering thermoelastic deformation associated with