

Nonlinear Mechanics of Crystals

SOLID MECHANICS AND ITS APPLICATIONS

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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.

John D. Clayton
Aberdeen, Maryland, USA
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