UNIFIED CONSTITUTIVE EQUATIONS FOR CREEP AND PLASTICITY

Edited by

ALAN K. MILLER

ELSEVIER APPLIED SCIENCE
World Publishing Corporation

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ELSEVIER APPLIED SCIENCE PUBLISHERS LTD
Crown House, Linton Road, Barking, Essex IG11 8JU, England

Sole Distributor in the USA and Canada
ELSEVIER SCIENCE PUBLISHING CO., INC.
52 Vanderbilt Avenue, New York, NY 10017, USA

WITH 11 TABLES AND 92 ILLUSTRATIONS

British Library Cataloguing in Publication Data

Unified constitutive equations for creep and plasticity.
1. Plasticity
I. Miller, A.K.
620.1'1233 TA418.14

Library of Congress Cataloging-in-Publication Data

Unified constitutive equations for creep and plasticity.

Includes bibliographies and index.
1. Deformations (Mechanics)—Mathematical models.
2. Materials—Creep—Mathematical models. 3. Plasticity—Mathematical models.
I. Miller, A. K. (Alan K.)
TA417.6.U55 1987 620.1'123'0724 87-8895

ISBN 1-85166-087-9
ISBN 7-5062-0418-[illegible]

Preface

Constitutive equations refer to 'the equations that constitute the material response' at any point within an object. They are one of the ingredients necessary to predict the deformation and fracture response of solid bodies (among other ingredients such as the equations of equilibrium and compatibility and mathematical descriptions of the configuration and loading history). These ingredients are generally combined together in complicated computer programs, such as finite-element analyses, which serve to both codify the pertinent knowledge and to provide convenient tools for making predictions of peak stresses, plastic strain ranges, crack growth rates, and other quantities of interest.

Such predictions fall largely into two classes: structural analysis and manufacturing analysis. In the first category, the usual purpose is life prediction, for assessment of safety, reliability, durability, and/or operational strategies. Some high-technology systems limited by mechanical behavior, and therefore requiring accurate life assessments, include rocket engines (the space-shuttle main engine being a prominent example), piping and pressure vessels in nuclear and non-nuclear power plants (for example, heat exchanger tubes in solar central receivers and reformer tubes in high-temperature gas-cooled reactors used for process heat applications), and the ubiquitous example of the jet engine turbine blade. In structural analysis, one is sometimes concerned with predicting distortion *per se*, but more often, one is concerned with predicting fracture; in these cases the information about deformation is an intermediate result *en route* to the final goal of a *life* prediction. In manufacturing analysis, one is more often concerned with predicting deformation response (such as press loads and die filling during forging) but is also sometimes concerned with predicting material failure (such as cracking during rolling and forging, tearing during sheet stretching and drawing, or fracture of metallic interconnects during integrated circuit fabrication).

Broadly speaking, the material phenomena pertinent to the above needs are governed by three physical processes: elastic deformation (stretching of interatomic bonds), non-elastic deformation (permanent switching of interatomic bonds among the various atoms in the solid), and decohesion (permanent breakage of bonds). The first process is predictable by the well-understood laws of elasticity and needs no further discussion in this book. The third category is so complex—because it depends not only on the material behavior at a point but also on the distribution of stresses and strains across the body—that few unified, generally applicable approaches for predicting fracture have emerged, other than the 'laws' of fracture mechanics which have well-known limitations. It is in the *second* category that the greatest progress has been made in the past several decades, in formulating equations that can predict the non-elastic deformation response under fairly general conditions; and this second category is the focus of the present volume.

The need to *predict* implies that the desired answer is not already available from experimental meaurements. In most cases, this is not because of a total lack of test data on the material of interest; it is because of the notorious history or path dependence of non-elastic deformation response. Even though experiments spanning the entire temperature and strain rate regime of interest may have been run, it is impossible to explore all of the sequences and combinations of loadings that might be imposed in service. Interactions of 'creep' and 'plasticity' are one such complication; non-proportional multiaxial deformation is a second. Thus, a major purpose of modern constitutive equations is to extrapolate from simple test data to complex histories. Of course, extrapolation in the usual sense, e.g. from short-term tests to long-term service, or from a small number of test data to all of the temperatures and strain rates of interest, is also a major objective of the constitutive equations presented herein.

The principle that extrapolation is most accurately done using equations founded on the actual governing physical processes has been invoked so often that it is scarcely necessary to mention it at this point. This principle gives us a practical, utilitarian reason for using as much as possible the scientific knowledge about non-elastic deformation in developing these constitutive equations. Chapter 1, drawing on its author's entire career in studying the physical mechanisms of non-elastic deformation, summarizes such knowledge. Most prominent among this knowledge is the fact that both 'plasticity' and 'creep' (at least creep due to slip) are controlled by the motion of dislocations; this leads directly to an obligation to *unify* 'plasticity' and 'creep' within a *single* set of equations, rather than taking the traditional engineering approach of one set of equations to predict 'time-independent plastic' strains and a separate set of equations to predict 'time-dependent creep' strains. Predicting both 'plasticity' and 'creep' within a single variable is the primary distinguishing feature of the unified constitutive equations approach.

Also prominent among our physical knowledge is the role of internal structure (e.g. dislocation density, state of internal stress, degree of solute clustering) in controlling non-elastic deformation. This leads directly to the use of internal structure variables, rather than only the external variables such as strain or time, to predict transient and steady-state responses with the unified equations.

Despite the fact that the above arguments make it incumbent upon us to try to simply *derive* a set of predictive equations from the actual physical mechanisms, it is impossible at the present time to do so. For one thing, despite the many great advances in our scientific knowledge about non-elastic deformation, the available 'first-principles' theories do not yet treat deformation under general loading histories, over wide ranges and changes in temperature, for multiaxial loadings, and in complex engineering materials. For another, even if they did, the resulting equations might be too cumbersome for structural or manufacturing analysis purposes. Faced with this situation, but still mindful of our obligation to build as much as possible of the physical knowledge into the equations, we are forced to make judgments of various sorts, such as:

- Which subset among all of the possible deformation phenomena deserves the most attention?
- Which types of internal variables should be used in the equations?
- Which are the most accurate quantitative expressions for predicting these phenomena?

As might be expected, various investigators differ in their judgments with respect to these and other factors. A natural consequence is the current existence of several unified constitutive equation approaches, all sharing a similar overall philosophy but differing in many details.

The major portion of this book (Chapters 2–6) is a presentation of five such approaches, each authored by its own 'proponent'. Chapter 1 includes elements of a sixth set of constitutive equations. The reader is invited to browse through this smorgasbord of approaches, both to develop an appraisal of the overall state-of-the-art in unified constitutive equations, and also to select the approach best suited to his or her own needs.

As an aid in assessing the merits (and a few demerits) of the various approaches, Chapter 7 discusses the equations presented in the earlier chapters. This critique is mostly from the point of view of a potential *user* of such equations, and focusses on both their predictive capabilities and their numerical behavior.

The above discussion has concentrated on the pragmatic aspects of unified constitutive equations as a methodology for engineering predictions. There is also a scientific accomplishment within these covers, namely partial progress towards a unified, first-principles model that can predict all aspects of non-elastic deformation behavior, based on a detailed representation of the internal physical processes. Clearly we are not there yet, but equally clearly, the field is closer to that goal with unified constitutive equations than it has been with the previous 'traditional' approaches. Perhaps it is not too unrealistic to hope that some future edition may present *the* universally-accepted, first-principles based, set of unified constitutive equations for plastic deformation and creep of engineering alloys.

It is a pleasure to acknowledge assistance from a number of sources. First and foremost are the authors who have contributed chapters to this endeavor. Collectively, they represent a clear majority of the expertise in this field. The staff at Elsevier Applied Science Publishers have been most helpful. Ms Virginia Sills provided considerable assistance in the preparation and coördination of the book manuscript. Other individuals, acknowledged by the authors of each chapter, were equally helpful. Many agencies provided financial support for the sponsored research programs under which the constitutive equations presented herein were developed; these agencies are acknowledged in the individual chapters but special mention must be made of the US Department of Energy, Office of Basic Energy Sciences, Materials Sciences Division, which not only supported several of the individual efforts but also provided support for the Editor during the preparation of this book.

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Constitutive Behavior Based on Crystal Plasticity

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1. INTRODUCTION

Constitutive equations are the vehicle by which our knowledge of material behavior enters into engineering design. At the very least, they should be sufficiently accurate. This could be—and frequently is—achieved by an empirical description based on data obtained under conditions that essentially duplicate those of the specific application. Of more general usefulness are relations that can be applied under a wide range of conditions and for many materials, containing a number of materials parameters (the fewer the better), which can be measured in simple tests. Such general relations can be expected to be found only if they fulfill two conditions: they must be phenomenologically sound; and they should be based on as much of the underlying physics as can be ascertained with some confidence. The closer the phenomenological description reflects the actual physical processes involved, the further it can be extrapolated beyond the range of variables for which it was measured.

Phenomenological soundness reflects, *inter alia,* an appropriate choice of variables, and a formulation that exhibits the proper invariance against arbitrary frames of reference. For example, it recognizes that the material responds to stresses, not forces (thus separating parameters of the geometry from those of the material), and that the stress is a second-rank tensor; it takes proper account of the changes in geometry with finite deformations, usually by the use of matrix descriptions. These problems are by no means trivial, but they are solvable. More subtle are judgments as to whether one should use history or state variables, integral or differential descriptions, and the like.

We will address some of these questions briefly but will, in the main, oversimplify the phenomenological aspects in order to concentrate on the material properties. Thus, we will inquire into the behavior of a *material element* (a convected volume element) under a macroscopically uniform stress during a macroscopically uniform, *infinitesimal* increment of strain. These (local, average) stresses and strain-increments are supposed to be related to surface tractions and surface displacements by the standard methods of solid mechanics. For this purpose, the medium in which the element is embedded is considered non-dissipative—though the element itself is essentially dissipative. By this convention, the local stresses and strain-increments become, in effect, the 'applied' variables (regardless of which is viewed as the independent and which as the dependent one). Their product is the work done by the environment on the material element under consideration, representative, in the end, of the lowering of weights at the surfaces.[1]

We will regard the material element as being at *constant temperature,* on the time scale for which the behavior is described. The *material response* is then principally the relation between the stress and the strain-increment. In addition, the stress increment, time-rates of change, and other variables may enter under certain circumstances.

The prime lesson to be learned from materials science is that there is not one material response, one 'mechanical equation of state', or even one set of differential constitutive equations. If such a completely general formulation were attempted, it would be too complicated to be of any use. A more effective approach is to look for *classes of materials, regimes of variables,* and *aspects of behavior,* for which a 'universal' constitutive description can be found. For example, in the present treatise, we will concentrate on polycrystalline, single-phase metals of cubic lattice structure that have been plastically deformed by, say, 1–100%, at temperatures between about 20 K and one-half to two-thirds of the melting temperature, at strain rates between about 10^{-7} and $10^{3}\,s^{-1}$. Withing this restricted (though very broad) 'interest space', deformation is governed by *crystallographic slip* in the grains of the material element or, on a finer scale, by *dislocation glide* and *dislocation storage.* This assessment of the physical mechanisms allows one to formulate a meaningful set of stress/strain relations, with respect to both the kinetics and the multi-axial behavior.

An important input from an understanding of the physical mechanisms is the provision of *diagnostic tools* to assess whether a specific material under specific conditions in fact falls within the assumed 'regime'.[1,2] In Section 7 we will give some examples; in particular, it will be outlined how one can assess whether a material behaves, in its macroscopic properties, like a 'single-phase' or a 'multi-phase' material, which has important implications for the hardening rule to be expected.

A final decision one has to make is which *aspects of behavior* to include. Again, if one attempted to condense *all* aspects of the mechanical behavior into one general set of constitutive relations, these would quickly become unmanageable. This is the point in any complex problem where judgment becomes of paramount importance. For the purposes of the present treatise, considering the 'interest space' circumscribed above, it is our judgment that a sufficiently self-contained description of *plasticity* can be obtained by ignoring elasticity and anelasticity, unloading and reverse-loading effects, inertial effects and body-forces, and energy storage. We will give some justifications for this judgment in Section 2. The judgment concerns material properties only; for *calculational* purposes, an inclusion of elasticity is sometimes necessary (when pure plasticity relations cannot be inverted), and body forces are sometimes used explicitly as an algorithmic tool, etc.

Our primary concern will be with three aspects of material behavior:

- the *kinetics* of flow under the influence of thermal activation, which is well described elsewhere[1,3] and will only briefly be summarized in Section 3;
- the influence of polycrystal plasticity on the *multi-axial* stress–strain relations for *anisotropic* materials, for which we present new results in Section 4;
- the description of the *evolution* of the state parameters, which is given for both texture and substructure evolution in Section 5, including some new proposals for treating a specific second state parameter.

To round out these primary concerns, we will discuss various meanings of the term 'internal stress' in Section 6, and assess them with respect to the necessity or usefulness of introducing such an extra parameter. Finally, in Section 7, we summarize diagnostic procedures to establish the type of behavior that controls a given material in a given regime of the variables, and summarize the constitutive relations for the interest sphere emphasized in this article. This leads to some general recommendations in Section 8.

A recurring theme in constitutive relations is scaling laws. We will give some general guidance to various stress and temperature scaling parameters. In addition, we discuss briefly the fundamental question of *scale*: the size of a meaningful material element (Section 3.1.1).

A major theme of this book is 'unified' constitutive equations for 'plasticity' and 'creep'. In the physical theories of plastic deformation, this unification exists *ab initio*: whether the strain (rate) is prescribed and the stress is measured, or the stress is prescribed and the strain (rate) measured—the material response is the same, it must be independent of the boundary conditions.

The material response is also independent of the history; it is entirely determined by the current (micro-)structure, regardless of which path was taken to get there. This may be called the 'article of faith' of material scientists, and it will be assumed throughout this work: *current behavior depends only on the current state*. The current rate of evolution of the state is one aspect of current behavior.

2. SOME IMPORTANT REALITIES

For problems as complicated as plasticity, there is no hope of ever finding a 'correct' solution, from first principles, even for a restricted interest space. The most important decisions are made before one writes down the first equation: namely, what to consider important and what to neglect if necessary. It is not only approximations at the solution stage that are made (as anywhere in physics), but also judgments at the problem-setting stage. To be as wise as possible in making these judgments, it is imperative to have most of the basic realities in mind.

2.1. Uniaxial Monotonic Deformation

2.1.1. Yield

Figure 1(a) shows the beginning of a typical stress/strain curve. It is drawn on a scale that emphasizes the transition from elastic to plastic