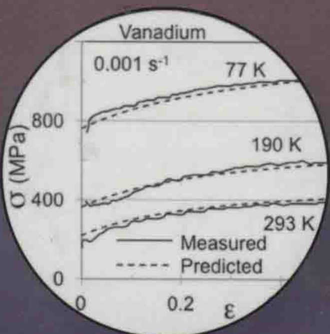
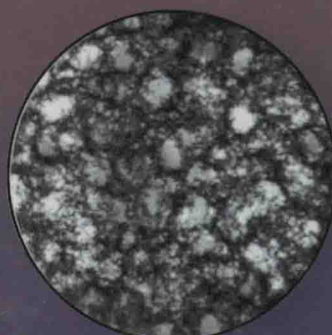
FUNDAMENTALS OF STRENGTH

Principles, Experiment, and Applications of an Internal State Variable Constitutive Formulation





PAUL S. FOLLANSBEE

Foreword by **George T. (Rusty) Gray III, Los Alamos National Laboratory**

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FUNDAMENTALS OF STRENGTH

FOREWORD

This monograph by Professor Paul S. Follansbee encompasses first an introduction to the elements controlling the mechanical behavior of metals; that is, crystal structure, thermodynamics, dislocations and twinning, defect–obstacle interactions, work hardening, deformation kinetics, and how the mechanical behavior of metals is quantified using mechanical testing. This book then provides an in-depth introduction as both a teaching aid to the faculty member and/or student to the mechanistic basis of an internal state variable-based constitutive model, specifically the mechanical threshold strength (MTS) model, as well as a seminal reference to professional researching and modeling the mechanical behavior of face-centered cubic (FCC), body-centered cubic (BCC), and hexagonal close-packed (HCP) metals and alloys. The thermodynamic and physical basis of the model's derivation is presented in detail as well as the evolution of the modeling approach to first treat pure metals, then alloys, and finally the complications imposed by multiphase alloys. The methodology of data requirements, data analyses, and the derivation of the different terms of the MTS model are summarized for a fictitious metal to illustrate the step-by-step procedures for the model construction.

Thereafter, three chapters of the monograph present detailed reviews of the application of the MTS model to FCC pure metals and alloys, followed by BCC metals and alloys, and finally, HCP metals and alloys where the complications of both deformation twinning and dynamic strain aging effects are discussed. Building upon the approaches set forth in the previous chapters, the author presents a chapter considering the deformation in austenitic stainless steels including both the effects of dynamic strain aging as well as the impact of irradiation damage on work hardening and deformation kinetics. Application of the model to the strength and deformation response of heavily deformed metals, such as that encountered during equal-channel angular pressing (ECAP) is described for a number of metals and alloys. Finally, a summary of the status of the MTS model and the challenges of additional physics requirements for internal state variable models to complex loading and processing paths is discussed.

This is an exceptional monograph for the student, faculty researcher or professor, and the experimental or theoretical and modeling researcher tasked with understanding the use of physically based predictive constitutive models for metals and alloys written by the preeminent author of the MTS model.

George T. (Rusty) Gray III
Los Alamos National Laboratory

PREFACE

This monograph was compiled to accomplish several objectives. First, I have enjoyed the opportunity to work with undergraduate students at Saint Vincent College (SVC) in Latrobe, Pennsylvania, on projects related to deformation modeling in metals. While I teach an introductory materials course, I have found that each time I take on a student I have spent considerable time independently teaching the student about the basis of the mechanical threshold stress (MTS) constitutive model—an internal state variable formulation. I have found it necessary to review topics related to mechanical testing, crystal structure, thermodynamics, dislocation motion, dislocation–obstacle interactions, hardening through dislocation accumulation, and deformation kinetics. Thus, I chose to write this monograph so that information they needed would be available in a single source. This monograph touches upon some topics that are covered in much more detail in available introductory materials textbooks. The chapter on structure and bonding, for instance, introduces the student to interatomic forces and dislocations, because these are essential to the understanding of strength. However, the material is incomplete and is not intended to replace the level of coverage found in an introduction to materials engineering textbook.

A second objective has been to document as completely as possible the mechanistic basis of the MTS model. The model has been under development for 25 years and has experienced use and evolution by multiple investigators. I believed a monograph focused on the elements of the model would assist others in its application. To accomplish this, I have tried to be clear about parts of the model that are soundly based—and I attempt to describe this—and others that are based on less-sound assumptions. A chapter has also been included to instruct investigators how to develop MTS model constants. I created a fictitious metal—FoLLyalloy—to demonstrate the required experimental test matrix and how measurements are analyzed.

Finally, I have included numerous examples of model implementation. In most cases, data available in the open literature have been used. Often, data have been extracted from a published figure using a digitization protocol, followed by curve smoothing to remove digitization errors if the published curve is smooth. Experience suggests that the digitized data agree within 2% of the actual data. Analysis of published data is not intended to repeat work in the literature but to show how experience with the MTS model has evolved, how this experience has eased model implementation, and how the MTS model can be used to understand the effects of new strengthening mechanisms, for example, fine grain processing or irradiation damage, when deformation in the base alloy is well understood.

PAUL S. FOLLANSBEE

ACKNOWLEDGMENTS

Much of the work summarized in this monograph was performed at Los Alamos National Laboratory. Sig Hecker brought me there in 1981 to join the mechanical properties team and to develop a research program in dynamic deformation mechanisms and experimentation. In the mid-1980s, Sig created and led the Center for Materials Science (CMS) at Los Alamos and hired Fred Kocks, Terry Mitchell, and Ricardo Schwartz as permanent CMS staff. Along with the opportunity to interact with these experienced materials scientists, the CMS supported a Summer Research Group, which included preeminent scientists such as Mike Ashby, David Embury, John Hirth, John Hutchinson, Ali Argon, Heinz Mecking, Frans Spaepen, and Tony Evans. The annual opportunity to present my evolving research and receive feedback was invaluable.

I particularly recall one seminar given by John Jonas, McGill University, in the early 1980s. The title of this seminar was the perhaps blasphemous "Metallurgy by MTS." During this talk, John emphasized how much one can learn about a material and indeed its microstructure from a mechanical test. In a way, this monograph provides further support for this premise. Moreover, it is interesting to note how much impact a single seminar or professional interaction can have on an early career scientist.

The interactions with Fred Kocks over a 10-year period were intense and productive. Much of the theory that underpins the MTS model was developed by Fred and Heinz Mecking. My contribution was a thorough experimental program that endeavored to measure the state variables and their evolution in model (face-centered cubic [FCC]) metals and then to expand the modeling to more complex materials systems and processing histories.

It is impossible to acknowledge enough my professional collaboration and friendship with Rusty Gray. Rusty was brought to Los Alamos to develop a research program studying shock deformation. He quickly rose to lead the dynamic deformation research team and is recognized as one of the world's experts in this field. Members of his team, including Shuh-Rong Chen, Anna Zurek, John Bingert, Dick Hoagland, Ellen Ceretta, Carl Trujillo, Carl Cady, Bill Blumenthal, Mike Stout, Manny Lovato, Mike Lopez, and, over the years, many postdocs and graduate students made up an incredibly strong research group.

I have had many productive interactions with scientists all around the world. Yuri Estrin and I share a strong interest in physically based constitutive laws. The work led by Sia Nemat-Nasser at University of California, San Diego (UCSD) is of very high quality. I particularly enjoyed a chance to interact with this team during a 1987 sabbatical. I call attention to my discussions with Mark Meyers, Ron Armstrong, Paul Dawson, Rod Clifton, Amiya Mukerjee, Tony Rollett, Glenn Daehn, John Hack, K. T. Ramesh, Qiuming Wei, Yuntian Zhu, David Srolovitz, and many others.

I wish to thank Jim Williams who served as my mentor and thesis advisor at Carnegie Mellon University. He is a model for the melding of scientific depth with application in the materials discipline, which has been one objective of this monograph. Jim was an early supporter of this project and has offered much interest and encouragement.

I am grateful for the full support provided to me by Br. Norman Hipps, President of Saint Vincent College, Dr. John Smetanka, Vice President for Academic Affairs, and Steve Jodis, Dean of the Boyer School of Natural Sciences, Mathematics, and Computing. Saint Vincent College has provided me a wonderful environment for creating this monograph. I have also had the opportunity to work with several students on this project. Two of the chapters include work that comprised part of the undergraduate research projects of Frank McGrogan and Aaron Weiss. I acknowledge contributions from several Saint Vincent College students, including Caitlin Sawyer, who reviewed chapters and searched for typographical and other errors; Marley Case, who created several diagrams using AutoCAD®; and Ashlee Zaffina and Loren Ostrosky, who helped compile the index.

My wife, Carolyn, has fully supported my efforts on this project and has even helped with scanning and digitization of literature data and other tasks. I could not have completed this monograph without her partnership. My three children, David, John, and Nicole, have followed my progress with interest and support. I hope the completion of this project has provided a lesson on the achievement of challenging goals.

P.S.F.

HOW TO USE THIS BOOK

PAUL S. FOLLANSBEE

JAMES F. WILL
Professor of Engineering Science

Students and others who have not had an introductory materials engineering course and are unfamiliar with mechanical testing to measure strength will want to start with Chapter 1, since this introduces basic concepts of stress, strain, and strain rate. Then, they may wish to continue with Chapter 2, which provides basic information on crystal structure and interatomic forces. The concept of dislocations is also introduced. Basic knowledge of dislocations is required before the reader can continue with Chapter 3, which provides an overview of basic strengthening mechanisms.

Those readers who are equipped with a working knowledge of the previously mentioned concepts and who are most interested in understanding the mechanical threshold stress (MTS) constitutive model may be able to begin with Chapter 4. This chapter discusses the dislocation–obstacle profile (variation of force versus distance moved) as the dislocation passes through a defected structure. It discusses features of this profile and the role played by thermal activation in deformation. Simple expressions for the temperature dependence of the yield stress are derived, and the importance of the yield stress at 0 K is emphasized. This chapter begins to compare model predictions with experimental data using simple kinetic analyses.

Chapter 5 introduces the basic MTS model—both the kinetic law and the hardening law. It discusses the path dependence that is observed in metal deformation and argues that a constitutive law needs to be able to follow path dependence.

Chapter 6 continues development of the MTS model by introducing various refinements that have been made to the basic development. Most important of these is the modification to the kinetic law to describe contributions from multiple strengthening mechanisms.

Chapter 7 demonstrates implementation of the MTS model through a fictitious metal—FoLLyalloy. With the desire to create a constitutive law for this alloy, the chapter leads the reader through the required experimental and analysis procedures.

Chapter 8 reviews work in copper, nickel, nickel–carbon alloys, and other alloys to illustrate application of the model in face-centered cubic (FCC) systems. In fact, the model has been most rigorously applied to these systems. Questions related to the treatment of multiple strengthening mechanisms are addressed. Also, the results demonstrate the temperature limit of the models developed to date.

The application of the model to body-centered cubic (BCC) pure metals and alloys is discussed in Chapter 9. Deformation in AISI 1018 steel, pure vanadium, and pure niobium is analyzed according to the procedures described for another fictitious alloy—UfKonel. Contributions of the Peierls obstacle are included as a second state variable, and complications introduced by deformation twinning and dynamic strain aging are discussed.

Chapter 10 addresses deformation in zinc, cadmium, magnesium, AZ31B (a magnesium alloy), zirconium, Zircaloy-2, titanium, and Ti-6Al-4V. The confounding contributions of deformation twinning and dynamic strain aging are analyzed from the standpoint of an internal state variable formulation.

Chapter 11 considers deformation in austenitic stainless steels. It applies methods developed in earlier chapters. The unique effect of nitrogen on strengthening in these systems is analyzed. Dynamic strain aging is again observed under certain conditions and this is analyzed in the same manner that was applied to hexagonal close-packed (HCP) and BCC metals in earlier chapters. The effect of irradiation damage on hardening and deformation kinetics is also discussed.

Chapter 12 introduces complications introduced by large-strain processing of metals, including texture effects and the stress dependence of the activation energy. Predictions of the model for ECAP-processed copper, nickel, stainless steel, and tungsten are compared to stress–strain measurements on the recovered, processed metals.

Chapter 13 offers a summary of the status of the MTS model formulation. Suggestions for further research are included.

Chapters 1 through 12 include exercises to assist the reader with the model application. Hypothetical data as well as actual literature data are used. Analyses of these data sets serve as practice for the student.

Solutions to the exercises are included in a Supplementary Web Site (http://www.wiley.com/go/fundamentals_excercises), which is available to all purchasers of this book. Many of the solutions involve spreadsheet analyses. Accordingly, the Supplementary Web Site includes Microsoft Excel© spreadsheets for each chapter. The worksheets in these spreadsheets are entitled by the exercise number. Readers will find in these spreadsheets the original versions of plots that have been copied into the Exercises Answers Chapter X.pdf files. Many of the exercises at the end of each chapter include tabular data. The .XLXS files conveniently place these data in a spreadsheet format for processing.

The initial worksheet in spreadsheet files for Chapters 7 and beyond is entitled "Model Parameters." This worksheet contains the specific MTS model parameters for the material noted in the exercise problem statement. The subsequent worksheets pull a specific model parameter when needed from the Model Parameters worksheet. Some of the spreadsheet files (e.g., Chapters 10 and 12) have a unique Model Parameter worksheet for each material considered. Users should use caution in changing parameters in individual cells. Cells are not password protected in these spreadsheets and it is possible to introduce errors that will plague the analyses.

LIST OF SYMBOLS

a	Length of a unit cell in a cubic crystal
A	Cross-section area (Eq. 1.1)
A_C	Parameter in temperature-dependent specific heat equation (Eq. 6.B5) (units: J/g/K)
A_{CS}	Constant in Equation (4.17) (units of T)
A_o	Model parameter in Equation (6.29) (units: MPa)
A_1	Model parameter in Equation (6.29) (units: MPa when $\dot{\varepsilon}$ is in units of s^{-1})
A_2	Model parameter in Equation (6.29) (units: MPa-$s^{-1/2}$)
b	Burgers vector
B	Parameter in temperature-dependent specific heat equation (Eq. 6.B5) (units: J/g/K^2)
c	Concentration (Eq. 3.10)
c_p	Heat capacity (Eq. 6.31)
C	Parameter in temperature-dependent specific heat equation (Eq. 6.B5) (units: J K/g)
d_{gs}	Grain size (Eq. 3.9)
D	Initial diameter of a test specimen
D_f	Final diameter of a test specimen
D_o	Constant in Equation (6.8) for the temperature-dependent shear modulus (unit: GPa)
E	Young's modulus (Eq. 1.5) (unit: GPa)
E_{app}	Apparent Young's modulus (Eq. 1.15)
E_{act}	Actual Young's modulus (Eq. 1.15)
F	Force

F_A	Attractive force between two ions (Eq. 2.1)
g_o	Normalized (and dimensionless) activation energy (Eq. 6.6)
g_{so}	Normalized (and dimensionless) value of A_{CS} (Eq. 6.7)
g_{oi}	Normalized activation energy representing a specific obstacle population (Eq. 6.18)
$g_{\varepsilon so}$	Model parameter in Equation (6.26) with subscript "ε" to emphasize interactions of dislocations with the stored dislocation density
G	Total activation energy in absence of stress assistance (Eq. 4.8)*
ΔG	Activation energy (Eq. 4.3)
k	Boltzmann's constant (1.38×10^{-23} J/K)†
k_c	Proportionality constant in Equation (3.10)
k_d	Proportionality constant in the Hall–Petch equation (Eq. 3.9)
K	Constant in the power law hardening equation (units of stress) (Eq. 5.1)
K_{DSA}	Proportionality constant in Equation (9.9) (unit: MPa^{-1})
K_{DSAo}	Constant in Equation (9.10) (unit: MPa^{-1})
K_S	Spring constant (Eq. 1.1) (units: N/m)
J_2	Second invariant of the stress deviator
L	Initial length of a test specimen
L_f	Final length of a test specimen
ΔL	Change in length (Eq. 1.4)
n	Exponent in the power law hardening equation (Eq. 5.1)
m	Strain-rate sensitivity (exponent in Eq. 5.3)
M	Taylor factor (Eq. 6.B3)
p	Exponent in Equation (6.9)—a more rigorous form of $\sigma(\hat{\sigma}, T, \dot{\varepsilon})$
p_i	Exponent p representing a specific obstacle population (Eq. 6.18)
r	Distance between two ions (Eq. 2.1)
q	Exponent in Equation (6.9)—a more rigorous form of $\sigma(\hat{\sigma}, T, \dot{\varepsilon})$
q_i	Exponent q representing a specific obstacle population (Eq. 6.18)
q_e	Electronic charge on an ion (1.602×10^{-19} C) (Eq. 2.1)
R	Gas constant (8.31 J/mol/K)
R_a	Atomic radius
R_d	Radius of a dislocation loop (Eq. 6.2)
s	Proportionality between σ and $\hat{\sigma}$ (Eq. 5.9)
S	Stiffness (Eq. 2.6)
S_o	Stiffness at the equilibrium separation distance between two ions
S_p	Spacing between precipitates (Eq. 3.15)
T	Temperature

* G also is used to represent the shear modulus, but the temperature T does not appear with G in these cases.

† k also is used in several equations as a constant (e.g., Eq. 2.1), but its use as Boltzmann's constant is most prevalent.