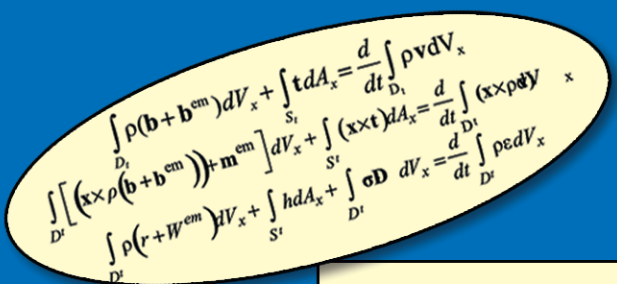
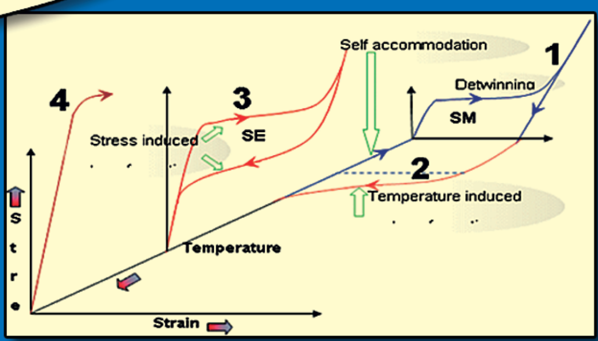
Modelling of Engineering Materials





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DEDICATION

The following close relatives and friends of the authors have left the mortal planes during the course of writing the current book. We dedicate this book to their inspiring memories.

.

To my grandfather

Krishnarao B. Deshpande

(4.8.1907 – 30.7.2008) – APD.

To my grandmother

Krovi Suryakantam

(15.7.1919 – 8.1.2009) – CLR.

To our friend and colleague

Devanathan Veeraraghavan (Dilip)

(28.9.1958 – 5.2.2009) – CLR & APD.

यस्याऽमतं तस्य मतं, मतं यस्य न वेद सः । (केनोपनिषत्)
Yasyāmatam tasya matam, matam yasya na veda saḥ (Kenopaniṣad)

For those who consider it to be not known, it is known. For those who claim to have known it, it is truly not known.

Preface

Engineers who are designing engineering systems using materials, often need a mathematical model that describes a material response, when a material is subjected to mechanical, thermal, electrical or other fields. Continuum mechanics attempts to provide the necessary mathematical framework that is useful in predicting the material response. *Continuum mechanics* is a classical as well as an emerging field that is exceedingly relevant to many researchers and practicing engineers in the fields of mechanical engineering, civil engineering, applied mechanics, chemical engineering and aerospace engineering among others.

Constitutive modeling is a topic that is part of continuum mechanics and is broadly understood by engineers as a phrase that deals with the equations that describe the response of a material sample, when it is subjected to external loads. In recent times, the term *constitutive model* is used to describe any equation that attempts to describe a material response, either during deformation or failure, independent of its origin or mathematical structure.

In the research community, *constitutive modeling* and *continuum mechanics*, involve investigations of physical mechanisms in materials and mathematical frameworks to describe them. Eventual goal of these researches is to describe macroscopic response of materials. Simulators and designers, on the other hand, are interested in using constitutive models in their simulations. These investigations are more focused on obtaining quantitative estimates of material behaviour. Reasonableness of physical mechanisms, correctness of mathematical framework, simplicity of mathematical models, ease of numerical simulations and reliability of estimates are all important aspects of modelling of engineering materials. In view of these issues involved in modeling of materials, the authors felt that a compilation and presentation of a broad review is necessary for the use of students, researchers and practicing engineers. This is attempted in the current book. The book has the following special features:

- It introduces the basic principles of continuum mechanics, so that the user is familiar with the mathematical tools that are necessary to analyze finite deformations in materials. Special care is taken to ensure that there is an engineering flavour to the topics dealt with in continuum mechanics and only the mathematical details that are necessary to appreciate the physics and engineering of a given problem, are highlighted.
- A brief review of popular linear material models, which are used in engineering, and which are derived based on infinitesimal deformation of materials, is presented in the book.
- Popular material models that are used to characterize the finite deformation of solids and fluids are described.
- Some examples of continuum characterization of failure in solids, such as modeling using plasticity theory, degradation parameter etc. are presented in this book.
- Principles behind the constitutive modeling of few modern special materials such as shape memory materials and ferroelectric materials are presented using the basic principles of continuum mechanics.
- Detailed case studies are presented which include a complete description of the material, its observed mechanical behaviour, predictions from some popular models along with a detailed discussion on a particular model.
- A brief overview of the tools that are available to solve the boundary value problems, is also given in this book.
- Detailed exercise problems, which will help students to appreciate the applications of the principles discussed are provided at the end of chapters.

The book is an outcome of the teaching of a course called *Constitutive Modelling in Continuum Mechanics*, by the authors at IIT Madras. The graduate students taking this course consist of new material modelers as well as material behaviour analysts and simulators. Majority of them, however, are involved in selection and use of material models in analysis and simulation. Therefore, main goal of the course has been to expose students with various backgrounds to basic concepts as well as tools to understand constitutive models. While teaching this course, the authors experienced the need for a book where principles of continuum mechanics are presented in a simple manner and are linked to the popular constitutive models that are used for materials. Hence, lecture notes were written to meet the course objective and these lecture notes are now compiled in the form a book.

The authors were inspired by a continuous exposure to the latest issues in the field of continuum mechanics, which was made possible through efforts by a leading expert in the field of continuum mechanics; Prof. K. R. Rajagopal, Professor of Mechanical Engineering, Texas A&M University. Prof. Rajagopal, kept the flame of interest in continuum mechanics alive at IIT Madras, through his regular involvement in workshops, seminars and discussions. The authors deeply acknowledge the inspiration provided by him to the authors, as well as to many other students and faculty at IIT Madras.

The authors place on record the contributions made by many of their faculty colleagues in the shaping of this book. Prof. Srinivasn M. Sivakumar, Department of Applied Mechanics at IIT Madras, provided us with the notes on plasticity, which formed the basis for the discussions on plasticity that is presented in Chapter 6. The authors thank him for his valuable help. Prof. Raju Sethuraman, Department of Mechanical Engineering at IIT Madras, provided the basic ideas for the review of numerical procedures, and was a constant source of inspiration for the authors in completing this book. We deeply acknowledge his encouragement and support. We acknowledge the help of Profs. Sivakumar and Sethuraman, along with Dr. Mehrdad Massoudi, U.S. Department of Energy, in formulating the contents of this book.

This book would not have been made possible but for the willing contributions of a number of M. S., Ph.D. and M.Tech students, who were working with us during their stay in IIT Madras. We also acknowledge all the students of the course over years, because class discussions and class projects were helpful towards formulating contents as well presentation of the book.

The illustrations were drawn with great enthusiasm by Mr. Jineesh George and Mr. Santhosh Kumar. The work of Dr. Rohit Vijay during dual degree project, formed the basis of the case study on asphalt that is presented in Chapter 5. Ms. K. V. Sridhanya's MS thesis formed the basis for the case study on soils that is presented in Chapter 6. Dr. S. Sathianarayanan, who worked on piezo-polymers for his Ph.D. thesis, has helped us to put together the discussion on piezoelectricity in Chapter 7. Efforts of Mr. N. Ashok Kumar, Mr. D. Pandit and Mr. M. Kishore Kumar, who worked on shape memory matrials for their theses, have helped us in compiling the material in Chapter 7. Rajesh Nair has taken the pains of going through parts of manuscript and pointing out some errors. Mr. V. Srinivasan helped us in the cover design of the book. Mr. Jose Vinoo Ananth, Mr. Mohammed Ghouse, Mr. G.G. Uday

Kumar, Mr. Suresh Kumar have also contributed in various capacities in bringing out the final form of the book.

One of the authors (CLR) has utilized his sabbatical leave that is granted by IIT Madras, towards writing the first draft of the book. We greatly acknowledge the support offered by IIT Madras for the encouraging atmosphere that it offers to pursue scholastic ambitions like writing a book.

Our publishers Ane Books Inc., were patient enough to wait from the submission of our original proposal to publish this book. We greatly appreciate their encouragement and patience in finally bringing out the final form of this book.

Last but not the least, the authors acknowledge the time spared by their family members and other friends, directly or indirectly, for encouraging the authors to pursue this project.

C. Lakshmana Rao

Abhijit P. Deshpande

Notations

Symbols style

Regular, italicized	scalar variables, components and invariants of tensors, material constants
Boldface, small	vectors
Boldface, capital and Greek	tensors
Boldface, italics	vector or tensor material constants
$\equiv$	definition
^	function
*	measurements made with reference to a moving frame of reference

Tensor operations

.	dot product involving vectors and tensors
$\times$	cross product involving vectors and tensors
ab, **vT**	dyadic product of vectors **a** & **b**, and vector **v** & tensor **T**
A:**B**	scalar product of tensors **A** and **B** (double dot product)
$\mathbf{A}^{\mathrm{T}}$	transpose of **A**
$\lvert\mathbf{a}\rvert$	magnitude of vector **a**
det **A**	determinant of **A**
tr(**A**)	trace of **A**
$\mathbf{A}^{-1}$	inverse of **A**

Derivative operations

$\dot{s}(X,t),\ \dot{v}(X,t),\ \dot{T}(X,t)$	total (material or substantial) derivative with respect to time
$\dfrac{\partial s(x,t)}{\partial t},\ \dfrac{\partial v(x,t)}{\partial t},\ \dfrac{\partial T(x,t)}{\partial t}$	partial derivative with respect to time

$\overset{\circ}{\mathbf{T}}$	rotational derivative of **T**
$\overset{\square}{\mathbf{T}}$	Jaumann derivative of **T**
$\overset{\Delta}{\mathbf{T}}$	lower convected or covariant derivative of **T**
$\overset{\nabla}{\mathbf{T}}$	upper convected or contravariant derivative of **T**
grad, div, curl	operators with respect to current configuration
Grad, Div, Curl	operators with respect to reference configuration
∇	gradient operator
∇^2	Laplace operator

List of symbols: Roman

A_x, A_X	areas in current and reference configuration, respectively
a	acceleration
B^r	reference configuration
b	body force
$\mathbf{b}^{em}$	electromechanical body force
B	$\mathbf{V}^2$, left Cauchy Green tensor or Finger tensor
$\mathbf{B}_t$	$\mathbf{V}_t^2$
C_{ij}	material parameter associated with strain energy density function
C	$\mathbf{U}^2$, right Cauchy Green tensor, matrix of elastic constants
C	stiffness coefficient
C^0	stiffness coefficient for biased piezoelectricity
$\mathbf{C}_t$	$\mathbf{U}_t^2$
$\mathbf{D}^v$	region (volume) in reference configuration
$\mathbf{C}^E$	electric current
D^r	Region (volume) in reference configruation
D^t	region (volume) in current configuration
D	stretching tensor (rate of strain tensor, symmetric part of the velocity gradient tensor)
$\mathbf{D}^E$	electric displacement
e	strain
e^e, e^p	elastic and plastic strain
e_p	accumulated plastic strain, locked-in strain
$\dot{e}$	strain rate at small deformations
E	enthalpy, Young's modulus

E_r	relaxation modulus
E^*, E', E''	complex, storage and loss modulus
E_1,E_2	Burger's model parameters
$\mathbf{e}$	infinitesimal strain tensor
$\mathbf{e^0}$	biased infinitesimal strain tensor
$\mathbf{e}_i$	set of orthogonal unit base vectors,
$\dot{\mathbf{e}}$	strain rate tensor at small deformations
$\mathbf{E}$	Green strain, Electric field
$\mathbf{E}_t$	relative Green strain
$\mathbf{E^E}$	electric field
$\mathbf{E^{E0}}$	biased electric field
f	yield function
$\mathbf{f}_i$	set of orthogonal base vectors in a rotating frame
$\mathbf{f}_t$	force acting on region D^t
$\mathbf{F}$	deformation gradient
$\mathbf{F}^e$, $\mathbf{F}^p$	elastic and plastic deformation gradient
$\mathbf{F}_t$	relative deformation gradient
G	shear modulus, Doi model parameter
$\mathbf{g}$, g	acceleration due to gravity
g_{ij}, g^{ij}	metric coefficients
$\mathbf{g}_i$, $\mathbf{g}^i$	set of generalized base vectors
h	surface source of heat
$\dot{H}_t$	rate of heating
$\mathbf{H}$	displacement gradient
$\mathbf{H_L}$	linear momentum
$\mathbf{H}_A$	angular momentum
i, j, k	dummy indices
$I_\mathbf{A}$, $II_\mathbf{A}$, $III_\mathbf{A}$	first, second and third invariants of tensor **A**, respectively
$\mathbf{I}$	unit tensor
J	Jacobian associated with **F**
J_c	creep compliance
K	power law model parameter
$\mathbf{L}$	velocity gradient
M	degradation parameter
m_{D^t}	mass of the body in the sub-region D^t
$\mathbf{m}$	unit tangential vector
$\mathbf{m}^{em}$	electromechanical body moment

M	total mass enclosed in a control volume D_t
$\mathbf{M}_t$	total moment
$\mathbf{n}$	unit normal vector
n	power law model parameter
N	number of cycles in cyclic plastic models
N_1, N_2	first and second normal stress difference
p	pressure, material particle
p'	effective mean stress
$\mathbf{P}$	material polarization
q	effective deviatoric stress
q^i, q_i	set of generalised coordinates
Q	electric charge, state variable in plasticity
$\mathbf{q}$	heat flux vector
$\mathbf{Q}$	orthogonal tensor, state variables in plasticity
r	volumetric source of heat
R	radius of the yield surface in the octahedral plane
$\mathbf{R}$	rotation tensor
$\mathbf{R}_t$	relative rotation tensor
s	distance, length
s_v	kinetic variable
S^r	area in reference configuration
S^t	area in current configuration
$\mathbf{s}$	1st Piola Kirchhoff traction
$\mathbf{S}$	1st Piola Kirchhoff stress
$\mathbf{S}_1$	2nd Piola Kirchhoff stress
t	current time
t^r	time at which material body takes B^r
t'	observation of time from a moving reference frame
$\mathbf{t}$	traction
u	pore pressure in soil mechanics
$\mathbf{u}$	displacement vector
$\mathbf{U}$	right stretch tensor
$\mathbf{U}_t$	relative right stretch tensor
V_x, V_X	volumes in current and reference configurations, respectively
v	volumetric strain
$\mathbf{v}$	velocity vector

$\mathbf{v_p}$	velocity of an object (projectile, particle etc.)
$\mathbf{V}$	left stretch tensor
$\mathbf{V}_t$	relative left stretch tensor
W	strain energy density
w_p	plastic work
$\dot{W}$	rate of work
$\dot{W}^{em}$	electromechanical rate of work
$\mathbf{W}$	spin tensor (vorticity tensor, skew-symmetric part of the velocity gradient)
$\mathbf{x}$	current configuration of a material point, representation of amaterial particle in real space
$\mathbf{x}'$	observation of the vector **X** from the moving reference frame
$\mathbf{x}^t$	configuration of a material point at time *t*
$\mathbf{X}$	reference configuration of a material point
y_i	set of orthogonal coordinates

List of symbols: Greek

α	scalar quantity
α_n	Ogden's material parameter
δ_{ij}	Kronecker delta
ε_{ijk}	alernator, alternating tensor
ε	internal energy
$\boldsymbol{\varepsilon}$	piezo electric coeficient matrix
$\boldsymbol{\varepsilon^0}$	piezo constant
$\in_0$	vacuum permittivity
ϕ	electric potential
γ	strain, shear strain
$\dot{\gamma}$	strain rate
η	entropy, stress ratio in soil mechanics
$\eta_1.\eta_2$	Burger's model parameters
κ	bulk modulus, mapping function between abstract and real configurations
κ_v	kinematic variable
κ	conductivity, dielectric constant
$\boldsymbol{\kappa^0}$	dielectric constant
λ	stretch or extension ratio, Lame's parameter, bulk or dilatational viscosity, plastic multiplier, structural parameter

λ_i	eigenvalues
μ	viscosity, Lame's parameter, Doi model parameter
μ_s	coefficient of static friction
$\overset{*}{\mu}, \mu', \mu''$	complex viscosity, real and imaginary parts of viscosity
μ_{n}	Ogden's material parameter
ν	Poisson's ratio
θ	temperature
θ_g	glass transition temperature
$\theta_l, \theta_h, \theta_{vh}$	low, high and very high temperatures to describe shape memory effect
ρ	density
σ_y	yield stress
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\boldsymbol{\sigma}'$	effective stress in soil mechanics
τ	relaxation time, time, Doi model parameter
τ_{ret}	retardation time
$\boldsymbol{\tau}$	deviatoric stress tensor
ω	angular frequency
$\boldsymbol{\omega}$	infinitesimal rotation tensor
$\boldsymbol{\Omega}$	body spin tensor
ξ	internal variable
ψ	Helmholtz free energy
ζ	Gibbs free energy

List of symbols: Script

$\mathscr{B}$	body in abstract space
$\mathscr{E}$	Euclidean space
$\mathscr{p}$	material particle in abstract space
$\mathscr{R}$	real space

Contents

CHAPTER

1 Introduction

आत्मा वा इदमेक एवाग्र आसीत्, नान्यत् किञ्चन मिषत् । (ऐतरेयोपनिषत्)
ātmā vā idameka evāgra āsit, nānyat kincana miṣat ... (Aitareyopanisad)

This existed as self-alone in the beginning. Nothing else winked.

1.1 INTRODUCTION TO MATERIAL MODELLING

All engineering materials are expected to meet certain performance requirements during their usage in engineering applications. These materials are often subjected to complex loadings, which could be in the form of a mechanical loading, a thermal loading, an electrical loading etc. or a combination of them. The response of the material to these loadings will determine the integrity of the material or the system in which the material is being used. A quantitative assessment of the material response when it is subjected to loads is very important in engineering design. This is possible if we have a mathematical description of the material response and its integrity, which can be called as a *material model.* The mathematical description of the system response, in the form of governing equations and boundary conditions, can be called as a *systems model.*

A model attempts to capture the underlying principles and mechanisms that govern a system behaviour through mathematical equations and is normally based on certain simplifying assumptions of the component behaviour. A model can typically be used to simulate the material as well as the system under different conditions, so as to predict their behaviour in situations where experimental observations are difficult. It is worth noting that in practice, we may have models that have a mathematical form without an understanding of physics, or models that describe the physics of the system, but may not be expressed in a specific mathematical form.