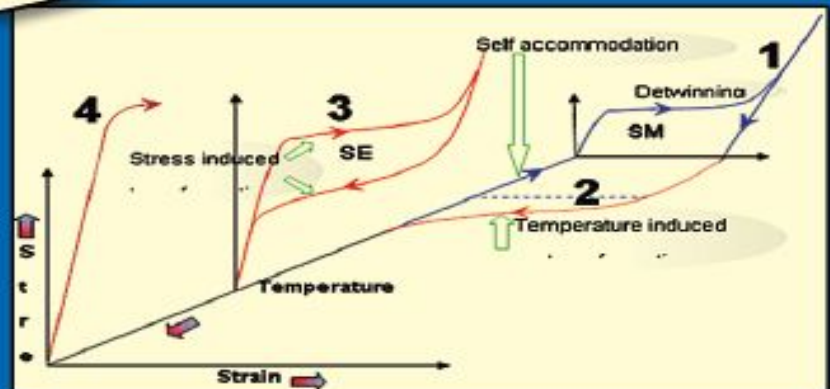


# Modelling of Engineering Materials

$$\int_{D^t} \left[ (x \times \rho(b + b^{cm})) + m^{cm} \right] dV_x + \int_{S^t} t dA_x = \frac{d}{dt} \int_{D^t} \rho v dV_x$$

$$\int_{D^t} \rho(r + w^{cm}) dV_x + \int_{S^t} h dA_x + \int_{D^t} \sigma D dV_x = \frac{d}{dt} \int_{D^t} \rho e dV_x$$



C Lakshmana Rao  
Abhijit P Deshpande

# Contents

[Preface](#)

[Notation](#)

[Chapter 1 Introduction](#)

[1.1 INTRODUCTION TO MATERIAL MODELLING](#)

[1.2 COMPLEXITY OF MATERIAL RESPONSE IN ENGINEERING](#)

[1.3 CLASSIFICATION OF MODELLING OF MATERIAL RESPONSE](#)

[1.4 LIMITATIONS OF THE CONTINUUM HYPOTHESIS](#)

[1.5 FOCUS OF THIS BOOK](#)

[Chapter 2 Preliminary Concepts](#)

[2.1 INTRODUCTION](#)

[2.2 COORDINATE FRAME AND SYSTEM](#)

[2.3 TENSORS](#)

[2.4 DERIVATIVE OPERATORS](#)

[Chapter 3 Continuum Mechanics Concepts](#)

[3.1 INTRODUCTION](#)

[3.2. KINEMATICS](#)

[3.4 CONSTITUTIVE RELATIONS](#)

[Chapter 4 Linear Mechanical Models of Material Deformation](#)

[4.1 INTRODUCTION](#)

[4.2 LINEAR ELASTIC SOLID MODELS](#)

[4.3 LINEAR VISCOUS FLUID MODELS](#)

[4.4 VISCOELASTIC MODELS](#)

## [Chapter 5 Non-linear Models for Fluids](#)

[5.1 INTRODUCTION](#)

[5.2 NON-LINEAR RESPONSE OF FLUIDS](#)

[5.3 NON-LINEAR VISCOUS FLUID MODELS](#)

[5.4 NON-LINEAR VISCOELASTIC MODELS](#)

[5.5 CASE STUDY: MECHANICAL BEHAVIOUR OF ASPHALT](#)

## [Chapter 6 Non-linear Models for Solids](#)

[6.1 INTRODUCTION](#)

[6.2 NON-LINEAR ELASTIC MATERIAL RESPONSE](#)

[6.3 NON-LINEAR INELASTIC MODELS](#)

[6.4 PLASTICITY MODELS](#)

[6.5 CASE STUDY OF CYCLIC DEFORMATION OF SOFT CLAYEY SOILS](#)

## [Chapter 7 Coupled Field Response of Special Materials](#)

[7.1 INTRODUCTION](#)

[7.2 ELECTROMECHANICAL FIELDS](#)

[7.3 THERMOMECHANICAL FIELDS](#)

## [Chapter 8 Concluding Remarks](#)

[8.1 INTRODUCTION](#)

[8.2 FEATURES OF MODELS SUMMARIZED IN THIS BOOK](#)

[8.3 CURRENT APPROACHES FOR CONSTITUTIVE MODELLING](#)

[8.4 NUMERICAL SIMULATION OF SYSTEM RESPONSE USING CONTINUUM MODELS](#)

[8.5 OBSERVATIONS ON SYSTEM RESPONSE](#)

[8.6 CHALLENGES FOR THE FUTURE](#)

[Appendix General and Convected Coordinates](#)

[Bibliography](#)

[Index](#)

# Modelling of Engineering Materials

**C. Lakshmana Rao**

*Faculty in the Department of Applied Mechanics  
Indian Institute of Technology (IIT), Madras*

&

**Abhijit P. Deshpande**

*Faculty in the Department of Chemical Engineering  
Indian Institute of Technology (IIT), Madras*

WILEY



Ane Books Pvt. Ltd.

**This edition published in 2014**

© (2010) C. Lakshmana Rao and Abhijit P. Deshpande

*Published by*

**Ane Books Pvt. Ltd.**

4821 Parwana Bhawan, 1st Floor

24 Ansari Road, Darya Ganj, New Delhi -110 002, India

Tel: +91 (011) 2327 6843-44, 2324 6385

Fax: +91 (011) 2327 6863

e-mail: [anebooks@vsnl.net](mailto:anebooks@vsnl.net)

Website: [www.anebooks.com](http://www.anebooks.com)

*For*

**John Wiley & Sons Ltd**

The Atrium, Southern Gate

Chichester, West Sussex

PO19 8SQ United Kingdom

Tel : +44 (0)1243 779777

Fax : +44 (0)1243 775878

e-mail : [customer@wiley.com](mailto:customer@wiley.com)

Web : [www.wiley.com](http://www.wiley.com)

***For distribution in rest of the world other than the Indian sub-continent***

ISBN : 978-1-118-91911-8

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, except as permitted by the UK Copyright, Designs and Patents Act 1988, without the prior permission of the publisher.

Designations used by companies to distinguish their products are often claimed as trademarks. All brand names and product names used in this book are trade names, service marks, trademarks or registered trademarks of their respective owners. The publisher is not associated with any product or vendor mentioned in this book.

*Library Congress Cataloging-in-Publication Data*

A catalogue record for this book is available from the British Library.

Printed at: Thomson Press, India

## **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. Mehرداد 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 materials 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 Ghose, 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
$\wedge$	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
<b>ab, vT</b>	dyadic product of vectors <b>a</b> & <b>b</b> , and vector <b>v</b> & tensor <b>T</b>
<b>A:B</b>	scalar product of tensors <b>A</b> and <b>B</b> (double dot product)
<b>A<sup>T</sup></b>	transpose of <b>A</b>
<b> a </b>	magnitude of vector <b>a</b>
<b>det A</b>	determinant of <b>A</b>
<b>tr(A)</b>	trace of <b>A</b>
<b>A<sup>-1</sup></b>	inverse of <b>A</b>

## Derivative operations

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

$\frac{\partial s(x,t)}{\partial t}, \frac{\partial v(x,t)}{\partial t}, \frac{\partial T(x,t)}{\partial t}$  partial derivative with respect to time

$\overset{\circ}{\mathbf{T}}$  rotational derivative of **T**

$\overset{\circ}{\mathbf{T}}$  Jaumann derivative of **T**

$\overset{\circ}{\mathbf{T}}$  lower convected or covariant derivative of **T**

$\overset{\circ}{\mathbf{T}}$  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

$\nabla$  gradient operator

$\nabla_2$ 

Laplace operator

**List of symbols: Roman**

$A_X, A_X$	areas in current and reference configuration, respectively
<b>a</b>	acceleration
$B^r$	reference configuration
<b>b</b>	body force
$\mathbf{b}^{\text{em}}$	electromechanical body force
<b>B</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
<b>C</b>	$\mathbf{U}^2$ , 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 configuration
$D_t$	region (volume) in current configuration
<b>D</b>	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
<b>e</b>	infinitesimal strain tensor
$\mathbf{e}^0$	biased infinitesimal strain tensor
$\mathbf{e}_i$	set of orthogonal unit base vectors,
$\dot{e}$	strain rate tensor at small deformations
<b>E</b>	Green strain, Electric field
	relative Green strain



$\mathbf{E}_t$	
$\mathbf{E}^E$	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
$\mathbf{g}_j, \mathbf{g}^i$	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 $\mathbf{A}$ , respectively
$\mathbf{I}$	unit tensor
$J$	Jacobian associated with $\mathbf{F}$
$J_c$	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
$q_i, q_j$	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

<b>W</b>	spin tensor (vorticity tensor, skew-symmetric part of the velocity gradient)
<b>x</b>	current configuration of a material point, representation of a material particle in real space
<b>x'</b>	observation of the vector <b>X</b> from the moving reference frame
<b>x<sub>t</sub></b>	configuration of a material point at time <i>t</i>
<b>X</b>	reference configuration of a material point
<i>y<sub>j</sub></i>	set of orthogonal coordinates

## **List of symbols: Greek**

$\alpha$	scalar quantity
$\alpha_n$	Ogden's material parameter
$\delta_{ij}$	Kronecker delta
$\varepsilon_{ijk}$	alternator, alternating tensor
$\varepsilon$	internal energy
$\boldsymbol{\varepsilon}$	piezo electric coefficient matrix
$\boldsymbol{\varepsilon}^0$	piezo constant
$\varepsilon_0$	vacuum permittivity
$\varphi$	electric potential
$\gamma$	strain, shear strain
$\dot{\gamma}$	strain rate
$\eta$	entropy, stress ratio in soil mechanics
$\eta_1$	Burger's model parameters
$\eta_2$	
$\kappa$	bulk modulus, mapping function between abstract and real configurations
$\kappa_V$	kinematic variable
$\kappa$	conductivity, dielectric constant
$\boldsymbol{\kappa}^0$	dielectric constant
$\lambda$	stretch or extension ratio, Lamé's parameter, bulk or dilatational viscosity, plastic multiplier, structural parameter
$\lambda_j$	eigenvalues
$\mu$	viscosity, Lamé's parameter, Doi model parameter
$\mu_S$	coefficient of static friction
$\mu^*, \mu', \mu''$	complex viscosity, real and imaginary parts of viscosity
$\mu_n$	Ogden's material parameter
$\nu$	Poisson's ratio
$\theta$	temperature
$\theta_g$	glass transition temperature
$\theta_l, \theta_h$	low, high and very high temperatures to describe shape memory

$\theta_{vh}$	effect
$\rho$	density
$\sigma_y$	yield stress
$\sigma$	Cauchy stress tensor
$\sigma'$	effective stress in soil mechanics
$\tau$	relaxation time, time, Doi model parameter
$\tau^{ret}$	retardation time
$\tau$	deviatoric stress tensor
$\omega$	angular frequency
$\omega$	infinitesimal rotation tensor
$\Omega$	body spin tensor
$\xi$	internal variable
$\psi$	Helmholtz free energy
$\zeta$	Gibbs free energy

### **List of symbols: Script**

$\mathcal{B}$	body in abstract space
$\mathcal{E}$	Euclidean space
$\mathcal{A}$	material particle in abstract space
$\mathcal{R}$	real space

---

विद्या ददाति विनयं विनयात् याति पात्रताम् ।  
पात्रत्वात् धानमाप्नोति धानात् धर्मं ततः सुखम् ॥  
( सुभाषितम् )

*vidyā dadāti vinayam vinayāt yāti pātratām.  
pātratvāt dhanamāpnoti dhanāt dharmaṃ  
tataḥ sukham. (Subhāṣhitam)*

**Knowledge gives humility, humility begets maturity. Maturity begets wealth. Wealth (earned in this way) establishes order and yields happiness.**

---

# 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.

In what follows, we will outline the complexity of material and its response in engineering. Several modelling approaches, which attempt to understand and predict the material response, are also discussed briefly. In this overview, we will recollect many popular terms that are used in material modelling. These terms are italicized, without a definition at this stage. However, they will be defined more precisely in later chapters, along with concepts related to them.

## **1.2 COMPLEXITY OF MATERIAL RESPONSE IN ENGINEERING**

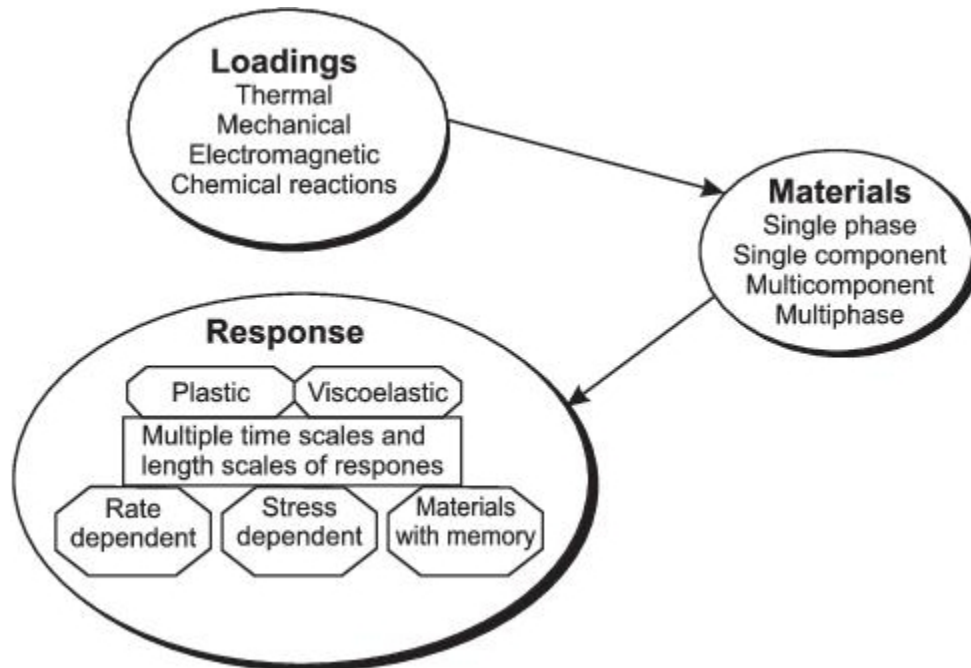
Materials that are currently being used in engineering, are fairly complex in their composition as well as in their response. Following are few examples of such materials. Many engineering materials are *heterogeneous* in their composition, since they consist of different components or phases. For example, any concrete is truly a heterogeneous material with aggregates and a matrix material like a cement paste or asphalt. Materials exhibit different response when they are loaded and tested in different

directions and hence are classified as *anisotropic*. Material composition can change through transformation *processes* such as chemical reaction and phase change. For example, a heterogeneous material may become homogeneous due to loading.

We will now outline few specific materials and their responses. Polymeric membranes, fiber reinforced composites are known to be anisotropic in their mechanical response. Many materials like polymers are '*viscoelastic*' in nature and exhibit a definite time dependent mechanical response. The same polymers show a time independent, large deformational response when they are deformed at temperatures above their '*glass transition temperature*'. We also know of the existence of special metals such as '*shape memory alloys*', which show drastic changes in their mechanical response when they are heated by about 50°C, causing a phase transition within the material. There are '*piezoelectric materials*' which are able to convert electrical energy to mechanical energy and *vice-versa*. Further, their electromechanical response is a function of the state of stress and the frequency of loading. Many engineering fluids show a '*linear stress-strain rate*' response, which is characterized by a parameter called as '*viscosity*'. However, there are other materials such as grease and paint, whose viscosity is dependent upon the state of stress at which the flow occurs. Blood clotting is a phenomenon where the material changes from a fluid to a solid. Mechanical response of blood during clotting can be understood only if biochemical reactions are also included in the model. The reasons for such complex material behaviour is also emphasized by analyzing *multiple time scales* of response and *multiple length scales* of response. The complexity of loadings, material make-up and its response is captured schematically in [Fig. 1.1](#).

**[Fig. 1.1](#)** Complexity of material response



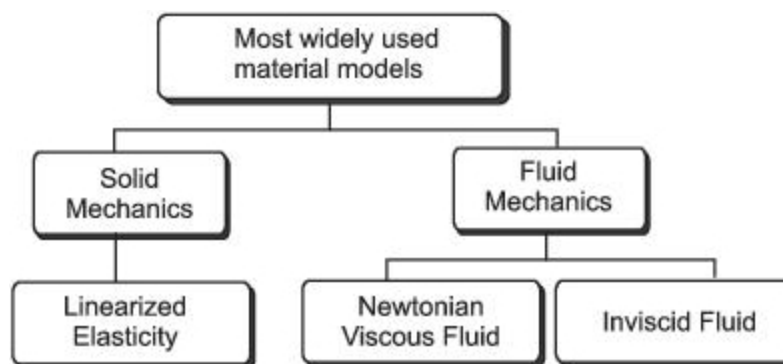


It is always desirable to capture all the features that are observations of material response through a mathematical model. Clearly, a mathematical model for any material that can accurately capture the response observed in experiments for any of the materials listed above, is quite complex. The mathematical model that we operate with, should reflect our own understanding of the material response. For example, we know from history of strength of materials that earlier attempts were made to correlate the load applied on any solid to the elongation experienced by it. It took about hundred years of evolution to prove that this attempt is faulty and correlations should really be found between a concept called *stress* which is defined as load per unit area and a concept called *strain*, which is the deformation per unit length. A further evolution led to the visualization of stresses and strains as *second order tensors*. An assumption that these two tensors are linearly related, led to a formulation that is popularly known as *linear elasticity*. Experimental observations on materials like rubber, proved that *load measures* like stress and the *deformation measures* like strain will not always be related

to each other linearly. The mechanical response of materials like rubber emphasized the need to introduce a *configurational (deformation)* dependence of stresses and the need for alternate deformational measures like *deformation gradients*. A redefinition of the *kinetic* (load related) measures and *kinematic* (deformation dependent) measures and their relationships are the main considerations in *continuum mechanics*. This framework is common to materials all classes of materials such as *solidlike, fluidlike* or gases.

It is worth noting that materials like metals and ceramics are clearly known to be *solids* and materials like water and oil are known to be *fluids*. Popularly, the response of solids has been considered through material model of linear elasticity. Similarly, the response of fluids has been considered through models of *Newtonian* or *inviscid fluid*. This is highlighted in [Fig. 1.2](#) in the form of most widely used material models. On the other hand, polymers and granular materials are known to exhibit features of both solids and fluids. Hence, the use of terms such as solidlike and fluidlike is necessary to describe the response of materials.

**Fig. 1.2** Most widely used material models that are studied as part of solid mechanics and fluid mechanics



Mathematical framework for the description of the state of a material is formulated based on abstract notions and quantities. Abstract quantities such as force, velocity, stress

and strain are used to define the state of a material. These quantities are visualized to be either scalars, vectors or tensors, having multiple components at any given point. However, experimental observations that can characterize the material, to the same detail as the mathematical framework, are generally not possible. For example, the only mechanical quantities that are measured for any material point are displacements and the time of observation. All other abstract quantities such as strains, velocities, accelerations, forces etc. are inferred from these basic observations. Consider, for example, experimental characterization of a piezo-electric material such as poly vinylidene flouride (PVDF). This material is primarily available and used in the form of thin sheets (25 - 100 mm). Testing of PVDF films in all the prescribed directions is not easy. Hence, often experimentalists perform some controlled experiments such as a uniaxial tension tests which provide data of load vs. longitudinal / transverse displacement. The constants that are demanded by a mathematical framework are often interpreted from the basic data collected from these simple tests. The interpretation of constants does lead a certain degree of uncertainty, since the interpretation of the same constant, for the same material, from two different tests may not always match with each other.

The mathematical models for any material can be assessed through comparisons with experimental observations. As mentioned above, these experimental observations are limited in nature. Hence, it is possible that there may be different mathematical models that are 'equally' successful in capturing the experimental observations. While it is necessary for a mathematical model to capture an experimentally observed phenomenon, this ability alone is not sufficient for the general applicability of the model in diverse situations. It is useful to classify

different modelling approaches that are used in engineering practice. These are outlined in the next section.

## 1.3 CLASSIFICATION OF MODELLING OF MATERIAL RESPONSE

Before discussing different modelling approaches, let us first look at a specific material response and multiple ways of analyzing it. It is known that if a plastic (polymer) sample is deformed and kept at constant extension, the force required to maintain the extension decreases with time. Therefore, it is said that the *stress is relaxing* and the experiment is termed as a *stress relaxation* experiment. Now, one could look at the load *vs* time data taken from different materials and observe that decreasing load can be described by functional forms such as exponential or parabolic. In this case, no hypothesis is made about the material behaviour and no detailed justification is given about why a particular functional form is chosen. The constants used in the functions will be different for different materials and can therefore be used to distinguish material behaviour. We will call such approaches to modelling of materials as empirical modelling.

Let us continue with our example and compare the response of the polymer in stress relaxation with other well known materials, such as steel or water. An observation can be made that the polymer response is in some way a *combination of the responses* of these two types of responses, namely elastic and viscous. Therefore, one can make hypothesis about material being viscoelastic and construct mathematical model, which in certain limits reduces to elastic or viscous behaviour. Such models will be

called phenomenological models, because the overall material response serves as a guide in building of the models. An example of such model is Maxwell model, which predicts that stress will decrease exponentially in a stress relaxation experiment. The constants used in the exponential form can be called *material constants* of Maxwell model, as they will be different for different materials.

With increasing theoretical development at the microscopic scale and computational resources, we can talk of another set of models, *i.e.*, *micromechanical models*. Such a model draws recourse to the make-up of material in its more elementary forms such as atoms, molecules, agglomerates, networks, phases etc. In our example of stress relaxation in a plastic, polymer would be considered as a collection of molecular segments. A hypothesis can be made about the mechanical response of a segment. The response of bulk polymer can be obtained if we are able to develop a mathematical model for a collection of polymer segments. Of course, such a model will also lead to decreasing stress at the bulk scale and material constants at the bulk scale.

More often than not, it is a combination of these approaches, empirical, phenomenological and microscopic, that is used by engineers to understand and predict material behaviour. Each of them is useful in a specific context. In the following discussion, we outline their strengths and limitations.

### **1.3.1 Empirical Models**

In engineering, many of the procedures and practices are also dictated by documents called *design codes and standards*. These documents are normally a compendium of human experience, documented for use by a practitioner with the least difficulty. In development of such documents,

all uncertainties and ambiguities in human experience, are also accounted for, so as to help to develop a *safe* design. Since the design codes are meant to be used by a common practitioner, they must necessarily use concepts that are more easily grasped by a common practitioner. The use of multiple components of stress tensor in all practical situations is difficult for a practitioner and hence, the three dimensional nature of stress is often captured in a convenient scalar stress measure such as an *equivalent stress*. Similarly, *equivalent uniaxial strain* measures are defined and sometimes a relation is sought between these defined equivalent measures. Even though these relationships may not have strict mathematical validity, they are useful in characterizing a material, especially when we want to characterize the material response due to complex time dependent loading conditions. We could call these equations as *empirical models*. The empirical models, by and large are curve fits of available experimental data. They will be very useful in design and are applicable within the range of data from which they have been derived. However, they have no basis in either the physics of deformation of the material, or in the mathematical rigor or accuracy of the variables that they are attempting to correlate. Such approaches are also adopted by researchers when they are handling new materials, whose response is not yet fully understood, and to obtain quick approximate description of material behaviour.

In recent times, an approach based on Artificial Neural Network (ANN) is being used to describe the material behaviour. A class of artificial neural networks, known as MLFFNN (Multilayer Feed Forward Neural Network) is being used to correlate the microstructural parameters with macroscopic mechanical behaviour. This ability of MLFFNNs is attributed to the presence of non-linear response units and the ability of the network to generalise from given