Robert A. Guyer and Paul A. Johnson

Nonlinear Mesoscopic Elasticity

The Complex Behaviour of Granular Media
including Rocks and Soil

WILEY-VCH Verlag GmbH & Co. KGaA

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Cover Picture
T. J. Ulrich, P. Johnson and R. A. Guyer, Investigating Interaction Dynamics of Elastic Waves with a Complex Nonliniear Scatterer Applying the Time Reversal Mirror, Phys. Rev. Lett., 98.10430 (2007)

Library of Congress Card No.: applied for
British Library Cataloguing-in-Publication Data: A catalogue record for this book is available from the British Library.
Bibliographic information published by the Deutsche Nationalbibliothek
The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available on the Internet at <http://dnb.d-nb.de>.

Printed in the Federal Republic of Germany
Printed on acid-free paper

Typesetting le-tex publishing services GmbH, Leipzig
Printing betz-druck GmbH, Darmstadt
Binding Litges & Dopf GmbH, Heppenheim

ISBN 978-3-527-40703-3

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Preface

Nonlinear mesoscopic elasticity (NME) is the identifier of a collection of extreme/unusual elastic behaviors. The purpose of this book is to describe these behaviors as seen in particular physical systems, to suggest generalization beyond the particular based on a simple picture of the underlying physics, and to provide an analysis/theoretical framework for assessment of behavior and for the description of experiments. Thus we begin here with a brief (so that those who realize they are in the wrong place find that out sooner rather than later) description of the physical systems that are candidates for NME; six examples are shown. The behaviors that are associated with NME are many; eight examples are shown. The physical state of NME systems is specified in a multidimensional space of parameters, for example, length scale, time scale, the size of stress/strain fields, the strength of internal forces, etc. The boundaries of this space are set. At the end of the following overview we will provide an outline of the book.

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2009

Nonlinear Mesoscopic Elasticity: The Complex Behaviour of Granular Media including Rocks and Soil. Robert A. Guyer and Paul A. Johnson

ISBN: 978-3-527-40703-3

Acknowledgements

We wish to acknowledge the contributions to this work by our many colleagues. These include our friends at Los Alamos National Laboratory, the Catholic University of Belgium, Turin Polytechnic Institute (Italy), University of Nevada at Reno (USA), Stevens Institute of Technology (USA), University of Paris East Marne-la-Vallée (France), University of Paris VI and University of Paris VII (France), the French Petroleum Institute, the Swiss Federal Institute of Technology (ETH), the Swiss Federal Laboratories for Materials Testing and Research (EMPA) Zurich (Switzerland), University of Le Mans (France), the National Oceanic Atmospheric Administration (USA), University of Mediterreanean (France), the Institute of Applied Physics (Russia), University of Maine (France), University of Stuttgart (Germany), and University of Massachusetts/Amherst (USA). We are grateful to the Institute of Geophysics and Planetary Physics at Los Alamos, the US Department of Energy, Office of Basic Energy Science and Los Alamos National Laboratory for their generous and ongoing support of this work.

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ISBN: 978-3-527-40703-3

1
Introduction

1.1
Systems

Figures 1.1 to 1.6 show six examples of systems that have NME: powdered aluminum, thermal barrier coating, sandstone, cement, ceramic, and soil. For each figure there is a scale bar or caption that makes it clear that the systems of interest have noticeable inhomogeneities on a length scale smaller than the sample size, say 100 μm, but much larger than the microscopic scale, 0.1 nm. We imagine the physical systems that possess NME to have *very approximately* a *bricks-and-mortar* character. The bricks [quartz grains in the case of rocks, packets of crystallites (quartz, feldspar, ...) with clay particles in the case of soils, single crystals of aluminum in the case of powdered aluminum, ...] interface with one another across a distinctive, elastically different system, the mortar (a system of asperities in the case of rocks, a system of fluid layers and fillets in the case of (wet) soil, a layer of defective material in the case of aluminum powder, etc.). We are interested in these systems on a length scale that is large compared to that of their bricks. Systems built up to this length scale have important elastic features conferred by the geometry of the system that are strikingly different from those of their bricklike constituents.

For example, in the case of a Berea sandstone, the typical elastic modulus is an order of magnitude smaller than the corresponding modulus of quartz, that is, the

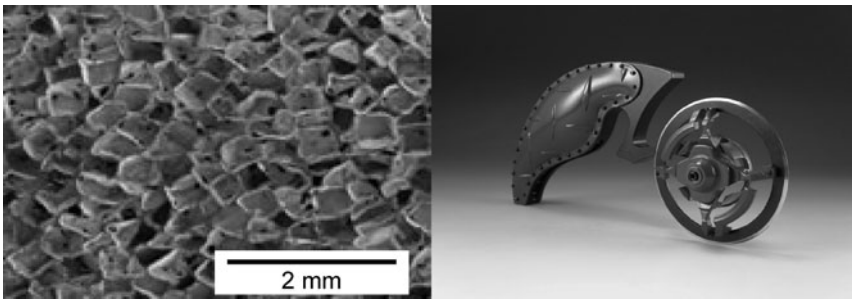

Fig. 1.1 Porous aluminum powder [9]. (Please find a color version of this figure on the color plates)

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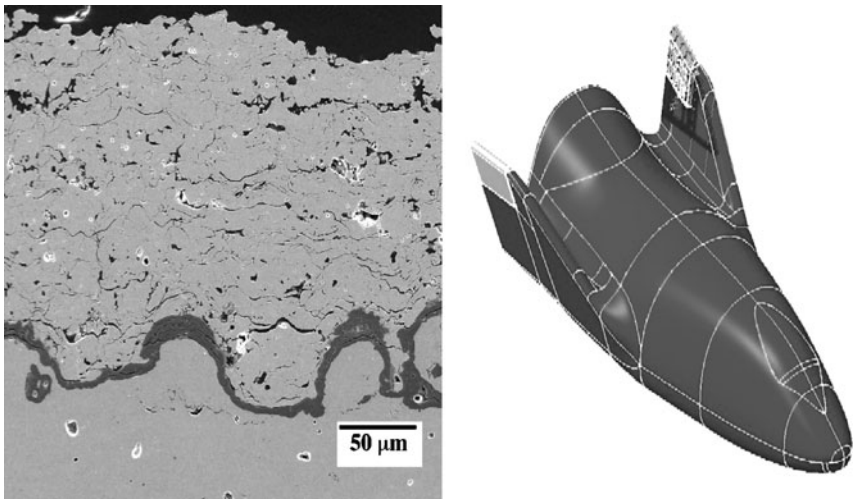

Fig. 1.2 Thermal barrier coating [10, 11]. (Please find a color version of this figure on the color plates)

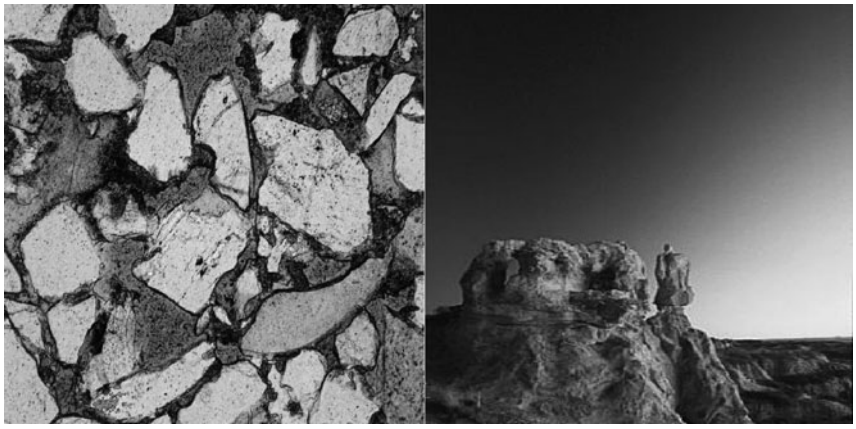

Fig. 1.3 Sandstone (typical grain size 100 µm) [12]. (Please find a color version of this figure on the color plates)

bricks. This means that a given force, say across a sample, produces ten times as much displacement as it would if applied across the quartz alone. This displacement must reside in the mortar as the assembly process could not have altered the stiffness of the bricks. The mortar is a minor constituent of the whole comprising, perhaps, 10% of the volume. Ten times as much displacement due to 10% of the volume means that the mortar is very soft and that it carries strains approximately two orders of magnitude greater than those in the bricks. Accompanying the inhomogeneity in the structure is an inhomogeneity in the strain. There is a further important point. Ten percent by volume of soft material randomly distributed in otherwise hard material could not markedly modify the response of the assembly.

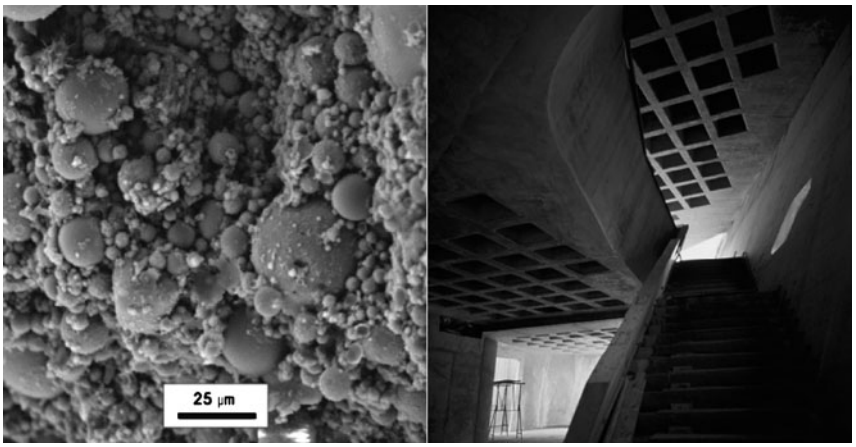

Fig. 1.4 Cement [13]. (Please find a color version of this figure on the color plates)

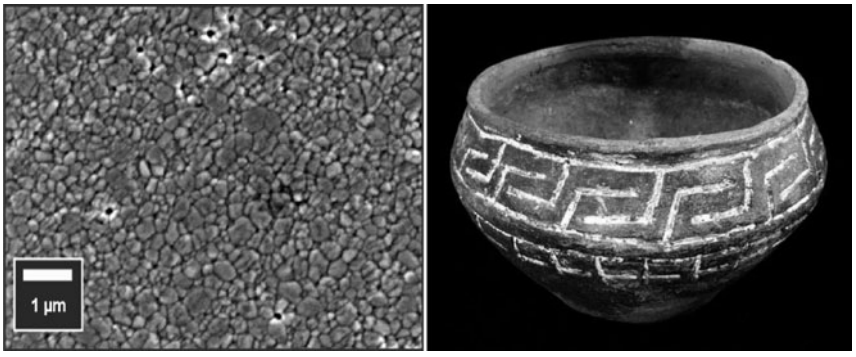

Fig. 1.5 Ceramic [14]. (Please find a color version of this figure on the color plates)

Fig. 1.6 Soil (sieved, typical grain size 1 mm) [15, 16]. (Please find a color version of this figure on the color plates)

The bricks-and-mortar picture captures an essential aspect of the way in which NME materials are constructed, that is, in such a way that the minority component (by volume) can effectively shunt the behavior of the majority component.

In identifying systems of interest with these simple ideas we cast a net that includes ceramics, soils, rocks, etc. But we do not pretend in any way to do justice to the disciplines of ceramic science, soil science, concrete science, ..., or even to elasticity in ceramics, soils, concretes, ... These are highly developed fields comprised of many subdisciplines. The discussion we present will be relevant more or less as dictated by the specific types of soil/ceramic/concrete/...

1.2 Examples of Phenomena

In Figure 1.7 we illustrate schematically eight examples of elastic behavior that we associate with NME. These include behavior that is quantitatively different from the usual behavior, behavior that is qualitatively different from the usual behavior, behavior that brings to the fore the importance of time scale and behavior in auxiliary fields. Not all NME materials possess these behaviors to the same degree. We sketch what is being illustrated schematically in each panel below. In the figure caption, information is given that locates an example of these experiments and characterizes them quantitatively.

1. The velocities of sound, c, of a sandstone are a factor of 2 to 4 less than those of the major constituent, for example, a quartz crystal. Thus the elastic constants of NME materials, K, $K \propto c^2$, might be less than the elastic constants of the parent material by an order of magnitude (even more for a soil).
2. When the pressure, P, is changed from 1 bar to 200 bar, the velocity of sound of a sandstone changes by a factor of 2. The same pressure change produces a 1% change in the velocity of sound in quartz (water, other homogeneous materials). Thus elastic nonlinearity, measured by $\gamma_c = \mathrm{d}\ln(c)/\mathrm{d}\ln(P)$, is very large for NME materials, often several orders of magnitude larger than that of the parent material.
3. When a sandstone (soil) is taken through a pressure loop, the strain that results is a hysteretic function of the pressure. In addition, when there are minor pressure loops within the major loop, the strain at the endpoints of the minor loop is "remembered". NME materials can have hysteretic quasistatic equations of state with endpoint memory.
4. A sample is subjected to a step in stress. Accompanying that step is a prompt step in strain followed by a slow further strain increase that evolves approximately as $\log(t)$. Recovery from the release of the step stress has a similar prompt step in strain and $\log(t)$ further reduction in strain. NME materials exhibit *slow dynamics* in response to transient loading.
5. The resonance of a bar of NME material is swept over at a sequence of fixed drive amplitudes. As the drive amplitude is increased, the resonant frequency shifts (to a lower frequency) and the effective Q of the system, measured by the amplitude at resonance, decreases. In a plot of the detected amplitude per unit drive, this is seen as a shift in the resonance peak accompanied by

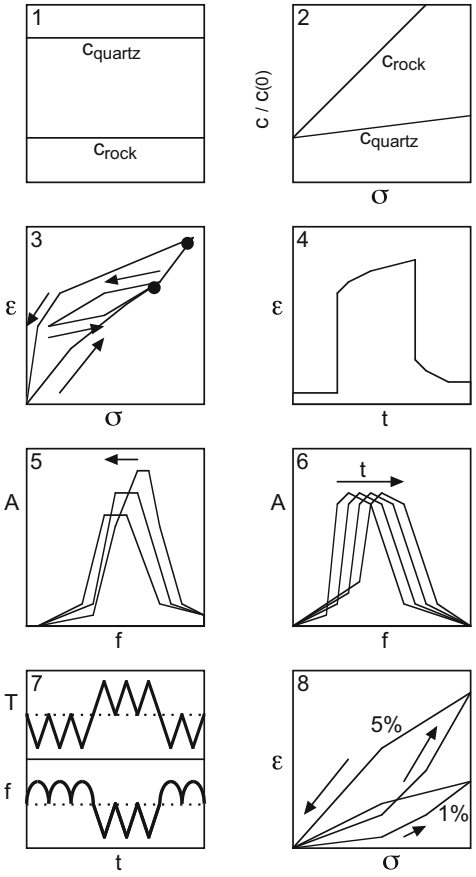

Fig. 1.7 Eight experiments. The eight experiments of interest are: (1) The velocity of sound, hence elastic constants, of a sandstone is a factor of 2 to 4 less than that of the major constituent, for example, a quartz crystal [1]. (2) When the pressure is changed, the velocity of sound of a sandstone changes by a factor of 2 for the application of 200 bar, whereas the same pressure change produces a 1% change in the velocity of sound in quartz (water, other homogeneous materials) [2]. (3) When a sandstone (soil) is taken through a pressure loop, the strain that results is a hysteretic function of the pressure and exhibits elastic endpoint memory [3]. (4) Accompanying the step in stress is a step in strain followed by a slow further strain response, that is, more strain, that evolves as $\log(t)$. Recovery from the release of the step stress has a similar strain step and $\log(t)$ further strain [4]. (5) The resonance of a bar of material is swept over at a sequence of fixed drive amplitudes. As the drive amplitude increases, the resonant frequency shifts (to lower frequency) and the effective Q of the system decreases [5]. (6) The slow evolution of the elastic state, brought about by an AC drive (compare to panel 4), can be seen in experiments in which the elastic state, once established, is probed by a low drive sweep over a resonance [6]. (7) When the temperature is changed slightly, the elastic response to that change involves a broad spectrum of time scales (compare to panels 4 and 6), suggesting $\log(t)$ behavior. In addition, the elastic response to temperature is asymmetric in the sign of the temperature change [7]. (8) A stress/strain loop similar to that in panel 3 is changed markedly by the configuration of fluid in the pore space [8].

a reduction of the amplitude at resonance. This behavior, which follows the fast motion of the drive, is an example of *fast dynamics*.

6. A bar of NME material is brought to steady state in response to a large-amplitude AC drive. The AC drive is turned off and the subsequent elastic state of the bar is probed with a low-amplitude drive that is swept over a resonance. The resonance, initially with resonance frequency shifted to a lower frequency as in panel 5, evolves back to a higher frequency approximately as $\log(t)$. The elastic state of the bar, established by a *fast dynamics drive*, relaxes once that drive is turned off by *slow dynamics*.
7. When the temperature of an NME material is changed slightly, the elastic response to that change, brought about by the temperature-induced internal forces, involves a broad spectrum of time scales (compare to panels 4 and 6), suggesting $\log(t)$ behavior at the longest times. In addition, the elastic response to temperature is asymmetric in the sign of the temperature change.
8. When an NME material is subjected to the internal forces of fluid configurations, a stress/strain loop similar to that in panel 3 is changed markedly. Much like a sponge, a rock is softer when wet.

The sequence of experiments sketched here call attention to the physical variables that are involved in the description of NME systems. The nature of a probe, the pressure, the temperature, the fluid configurations, the probe size, the duration of a probe, and the aftereffect of a probe having been present must all be considered and examined.

1.3 The Domain of Exploration

NME materials are probed in the complex phase space illustrated in Figure 1.8, that is:

1. Length. There are three length scales associated with NME materials, the microscopic scale (interatomic spacing) $a = 0.1\,\text{nm}$, the scale of inhomogeneity $b \approx 1\text{–}100\,\mu\text{m}$, and the sample size $L \gg b$. A quasistatic measurement is at $k \to 0$ ($k = 2\pi/\lambda$), whereas a resonant bar experiment is at wavelengths related to the sample size, $b \ll \lambda < L$.
2. Strain. There are judged to be two strain values of importance. At strains $\varepsilon < 10^{-7}\text{–}10^{-6}$, the nonlinear effects are small and have a more or less traditional behavior. At strains $\varepsilon > 10^{-3}\text{–}10^{-2}$ irreparable damage is done to a sample. The middle ground $10^{-7} < \varepsilon < 10^{-3}$ is the strain domain of NME.
3. Force. The standard for the strength of forces is the pressure given by a typical elastic constant, $K \approx \varrho c^2$, where ϱ is the density and c is the speed of sound, $K \approx 10^{11}\,\text{dyne/cm}^2 = 10^4\,\text{MPa}$ for a sandstone (1 atmosphere is $10^6\,\text{dyne/cm}^2 = 10\,\text{MPa}$). NME materials may be subject to a wide range of forces – applied forces, forces delivered to the interior of the systems from

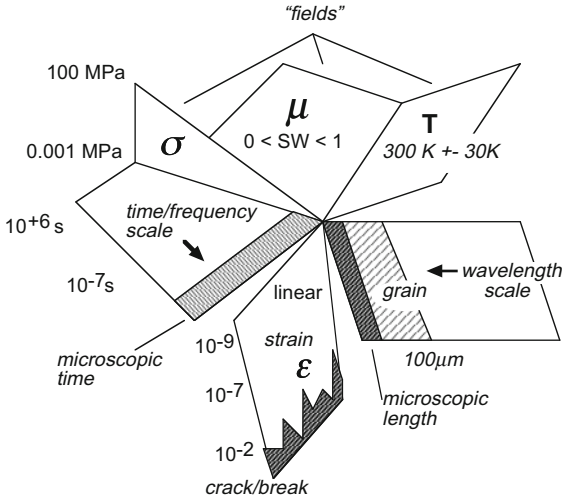

Fig. 1.8 Phase space. The materials of interest are probed on different time scales, length scales, and strain scales and with a variety of applied "fields".

the complex thermal response of constituents, or forces delivered to the interior of the system from arrangements of fluid in the pore space. The approximate strain consequence of a force (pressure) is found using $\varepsilon \approx P/K$, where P is the pressure. The strain range given above, $10^{-7} < \varepsilon < 10^{-2}$, implies 10^{-3} MPa $< P < 10^{2}$ MPa.

4. Time. The fastest time scale relevant to NME materials is approximately the time for sound to cross an inhomogeneity, $\tau \geq 100\,\mu\text{m}/c \approx 10^{-7}$ s. A resonant bar measurement is typically at 10^3–10^4 Hz (this scale is set by sample size L), a quasistatic measurement of stress/strain may last 10 min, and the strain response to a change in temperature may develop over a week. The range of time scales is enormous, 10^{-7} to 10^6 s.

All of these scales – length, time, and force – are far removed from the corresponding microscopic scales, for example, 0.1 nm is the microscopic length scale, 10^{12} Hz (a typical Debye frequency) is the microscopic time scale, and a microscopic energy per microscopic volume (say 0.1 eV/(0.1 nm)^3 ≈ 10 GPa) is the microscopic force scale (stated here in terms of pressure since force alone means little).

1.4 Outline

Our interest is in the nonlinear elasticity of mesoscopically inhomogeneous materials. We will discuss the theoretical apparatus that is used to describe these mate-

rials, the phenomenology of the experiments conducted, and the large body of data that illustrates the behavior that characterizes these materials.

In Part I, Chapters 1–5, we give a theoretical introduction to traditional linear and nonlinear elasticity. We begin the discussion at the microscopic level. It is here that the basic structure of linear and nonlinear elasticity is established and the numbers that determine the magnitude of almost all quantities of interest are set. It is a short step from a microscopic description to the continuum description that corresponds to the traditional theory of linear/nonlinear elasticity. These topics are covered in Chapter 2, which is followed, in Chapter 3, by a series of illustrations of the consequences of the theory. To get to the domain of elasticity of mesoscopically inhomogeneous materials we must jump a gap. Across this gap, where we will work, we start with a theoretical apparatus, having the same form as the traditional theory of linear/nonlinear elasticity, to which we will add a collection of *ad hoc* ingredients that have no immediate source in the domain we have left behind. A variety of mesoscopic elastic elements, contacts, interfaces, etc. are described in Chapter 4. So also is an effective medium scheme for turning mesoscopic elastic elements into elastic constants suitable for a theory of elasticity. The coupling of the elastic field to auxiliary fields, particularly temperature and saturation, is taken up in Chapter 5.

In Part II, Chapters 6–9, we introduce hysteretic elastic elements, or strain elements with an elaborate stress response, Chapter 6. The dynamics of elastic systems carrying these elastic elements can be complex because of an internal field that responds to stress slowly in time. A discussion of the resulting *fast* and *slow* dynamics is given in Chapter 7. A set of practical matters related to data analysis and modeling of data sets is taken up in Chapter 8. This is followed by a description in Chapter 9 of a wide variety of considerations that relate to using data on elastic systems for characterization (spectroscopy) and for location (tomography).

In Part III, Chapters 10–13, we discuss experiments. Quasistatic measurements, including coupling to auxiliary fields, are described in Chapter 10. Dynamic measurements, dynamic/quasistatic to dynamic/dynamic, are described in Chapter 11. The current picture of fast/slow dynamics is given a full airing. In Chapter 12, field experiments that touch on NME are described. The final chapter, Chapter 13, contains a description of a wide variety of nondestructive evaluation applications of NME.

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2
Microscopic/Macroscopic Formulation of the Traditional Theory of Linear and Nonlinear Elasticity

Following Section 2.1, in which we make a few observations that place the discussion of solids in the context of fluid/solid systems, there are two major sections. Section 2.2 starts with the description of microscopic elasticity and elaborates on the connection between the microscopic description of elasticity and the continuum description of elasticity, while Section 2.3 sets out the essentials of the continuum theory of elasticity, sans microscopic justification. (For those who want to skip over the foundations in Section 2.2, this is the place to start. Of course, one will have to be content to learn μ, λ, A, B, $\ldots$, β, $\ldots$ from experiments.) Many analytic details, Section 2.4, and some useful numbers, Section 2.5, are found at the end of the chapter.

In Section 2.2.1 we develop a description of the energy of a well-ordered solid, in terms of small displacements from equilibrium sites, which is the basis of the microscopic theory; in addition, we introduce the microscopic strains, etc. (Section 2.2.1.1). The dynamics of small displacements, due to forces caused by microscopic strains, leads to the phonon picture, the interacting phonon picture, etc. (Section 2.2.1.2). Some simple numerical estimates that tie microscopic numbers to macroscopic numbers are illustrated, for example, a linear elastic constant or a measure of the cubic anharmonicity. In Section 2.2.2, this mechanical (or quantum mechanical) description is married to an approximate but practical description of a solid in equilibrium with a temperature reservoir. In Section 2.2.2.1 we sketch the principle of the Gruneisen approximation, and in Section 2.2.2.2 we examine the resulting equations at reasonable temperatures, $T \approx 300$ K, and find the microscopic basis of other numbers, for example, the thermal expansion. We close Section 2.2 with a formal treatment of the microscopic description that results in the equations of continuum elasticity. Consequently, there is a microscopic link to the parameters of linear and nonlinear continuum elasticity, for example, μ, λ, A, B, $\ldots$, β, $\ldots$

In Section 2.3 we sketch the theory of linear and nonlinear continuum elasticity without recourse to a microscopic picture. The displacement field, strain, and stress are introduced, as is the elastic energy density, an analytic function of the strain field (Section 2.3.1). The dynamics of the displacement field are treated in Section 2.3.2. The coupling of the displacement field to auxiliary fields, temperature, saturation, $\ldots$ is described in Section 2.3.3. The generalization to inhomo-

Nonlinear Mesoscopic Elasticity: The Complex Behaviour of Granular Media including Rocks and Soil. Robert A. Guyer and Paul A. Johnson

ISBN: 978-3-527-40703-3

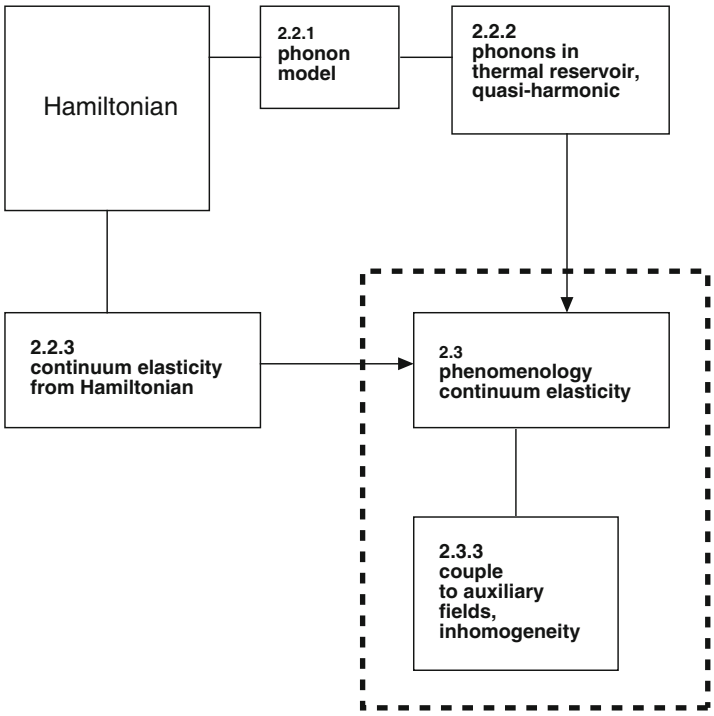

Fig. 2.1 Outline. The discussion in this chapter, from Hamiltonian to continuum elasticity, follows two routes, Sections 2.2.1 and Section 2.2.2, to the phenomenological model of elasticity. These routes supply some of the quantitative underpinnings of the phenomenological theory, which is able to stand on its own.

geneous elastic systems is made in Section 2.3.4 (see Figure 2.1). In Sections 2.4 and 2.5 details used in the chapter are provided.

2.1 Prefatory Remarks

First we step back from our immediate goal to look around. What distinguishes liquids and solids from gases at the atomic level is that in liquids and solids the particles (atoms or molecules) are **self-bound**. This means that the attractive forces between particles are sufficiently strong that they hold the particles near one another while the kinetic energy of the particles (their thermal motion, characterized by the temperature) causes them to move around, to attempt to fly apart. The particles in a gas are not self-bound; you have to put a gas of particles in a container with a lid to keep them together. To remove a particle from a liquid/solid you must reach

in and pull with a force strong enough to liberate it from its neighbors. The basic physical state of a collection of particles is determined by the ratio of the strength of the attractive forces, stated as an energy, and the energy of thermal motion, set by the temperature. Sometimes the thermal motions of the particles in a liquid/solid will conspire to deliver a large amount of kinetic energy to one particle and allow it to spontaneously leave the system, that is, evaporate.

And the difference between a liquid and a solid? It is one of degree and structure [1, 2]. In a solid the attractive forces between particles are sufficiently strong, compared to the disordering effect of the thermal motion, that a particular spatial arrangement of particles, each particle sitting advantageously in the attractive potential well of a regular array of neighbors, is the lowest energy state. The energy of a solid arrangement of particles differs from the energy of a liquid arrangement of particles by an amount that is small compared to the energy of either; the heat of fusion (roughly a measure of the energy difference between solid and liquid) is small compared to the heat of vaporization (by, say, a factor of 10 or so, the familiar 80 cal/g and 540 cal/g of freshman physics). The particles in a solid sit at well-defined places relative to their neighbors, and this local arrangement of particles is repeated again and again throughout space, that is, the solid, if it is a single crystal, has translational symmetry [3, 4]. Thus in a solid, where a particle should be is well defined; the departure of a particle from where it should be is also well defined. When you reach into a solid and pull a particle away from where it should be, its neighbors pull back. A set of internal forces arises in reaction to your pull with an accompanying set of displacements. The particle on which you are pulling is displaced and so are the particles that contribute the force trying to hold it in place. These are the manifestations of stress (the forces) and strain (the displacements) at the microscopic level. A description of what is happening at this level, a job for a chemist or a band structure physicist, involves looking at a material electron by electron, chemical bond by chemical bond.

2.2
From Microscopic to Continuum

2.2.1
A Microscopic Description

2.2.1.1 Microscopic Energy and Microscopic Strain

A crystal is an assembly of particles that to good approximation can be taken to reside near a set of lattice sites that are regularly arrayed in space. The symmetry of the crystal, for example, cubic, hexagonal, ..., describes the geometry of this regular array. Since the crystal is self-bound, it is characterized by atomic scale energies, forces, and lengths, ε_0, ε_0/a, and a, respectively, where a is the interparticle spacing. The typical particle is at a distance of a few Angstroms, tenths of a nanometer, from its neighbors and involved in an interparticle interaction of strength $\varepsilon_0 \approx 0.5\,\text{eV}$.

The forces between particles have strength ε_0/a of order 0.5 eV/0.1 nm or 0.1 nN (nanonewton) or 1000 K/Å or 0.1 (GPa)m^2. (The many units displayed here are a reminder that the measure of the importance of any energy/force is its size relative to another, for example, a photon energy in eV, a particle kinetic energy in Kelvin, an applied pressure in Pa, etc.)

The motion of particle R, at $\boldsymbol{x}_R$, near the lattice site with which it is associated, $\boldsymbol{R}$, is described by displacement $\boldsymbol{u}_R$, $\boldsymbol{x}_R = \boldsymbol{R}+\boldsymbol{u}_R$, and the corresponding momentum is $\boldsymbol{p}_R = m\dot{\boldsymbol{u}}_R$. The motion of particles away from their lattice sites is small. Typically at melting one has $|\boldsymbol{u}_R| \approx (0.20-0.25)a$ [5]. Thus particle motions are a small fraction of the intersite distance, and the energy of interaction among the particles can be developed as a series in the displacements, $\boldsymbol{u}_R$. For the energy in the assembly of particles we have

$$\mathcal{E} = \sum_R \frac{\boldsymbol{p}_R^2}{2m} + \frac{1}{2}\sum_R\sum_{R'} V(\boldsymbol{R}-\boldsymbol{R}'-\boldsymbol{u}_R+\boldsymbol{u}_{R'}) = \mathcal{K}+\mathcal{U}\,, \tag{2.1}$$

where $V(\boldsymbol{x}_{RR'})$ is the interaction energy between particles separated by $\boldsymbol{x}_{RR'} = \boldsymbol{x}_R - \boldsymbol{x}_{R'} \approx \boldsymbol{R}-\boldsymbol{R}'$, the equilibrium spacing between the lattice sites associated with the particles, Figure 2.2. Using $\Delta^\alpha = u_R^\alpha - u_{R'}^\alpha$ $(\alpha = x, y, z)$ we can write

$$\begin{aligned} V(\boldsymbol{x}_R-\boldsymbol{x}_{R'}) = \Phi_0(\boldsymbol{R}-\boldsymbol{R}') &+ \frac{1}{2!}\Phi_{\alpha\beta}(\boldsymbol{R}-\boldsymbol{R}')\,\Delta^\alpha\,\Delta^\beta \\ &+ \frac{1}{3!}\Phi_{\alpha\beta\gamma}(\boldsymbol{R}-\boldsymbol{R}')\,\Delta^\alpha\,\Delta^\beta\Delta^\gamma \\ &+ \frac{1}{4!}\Phi_{\alpha\beta\gamma\delta}(\boldsymbol{R}-\boldsymbol{R}')\,\Delta^\alpha\,\Delta^\beta\Delta^\gamma\Delta^\delta \\ &+ \ldots\,, \end{aligned} \tag{2.2}$$

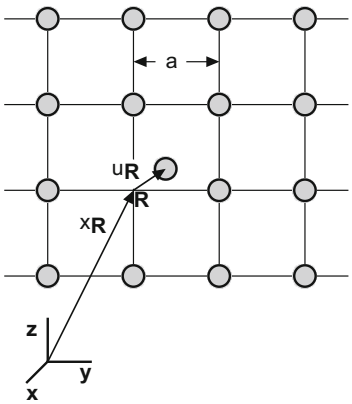

Fig. 2.2 Lattice. The set of vectors $\boldsymbol{R}$ and the displacements $\boldsymbol{u}_R$ allow one to track the particle at $\boldsymbol{x}_R = \boldsymbol{R}+\boldsymbol{u}_R$.