Chapter 1

Introduction

In this introductory chapter we explain first the main notions used in the book: waves, fronts, inhomogeneities, etc. and present some instructive examples which illustrate the topics. Then the outline of the book is described: theoretical considerations in the first part, followed by the analysis of one- and two-dimensional problems.

1.1 Waves and fronts

Waves and fronts are apparently similar. However, there are slight but essential differences between them in the admitted classical view. If waves essentially correspond to continuous variations of the states of material points representing a medium, then fronts are discontinuity surfaces (or lines) dividing the medium into distinct parts. But the shared characteristic feature of waves and fronts is their motion. The motion of waves and fronts is governed by the same governing equations, namely, by the fundamental conservation laws for mass, linear momentum, and energy in the standard cases. This is why we consider wave and front propagations under a single umbrella.

However, if these conservation laws (complemented by constitutive relations) are sufficient for the description of thermoelastic waves [Achenbach (1973); Graff (1975); Bedford and Drumheller (1994); Billingham and King (2000)], then for cracks or phase-transition fronts we need more. Certain additional relations are required in the presence of moving discontinuities in order to isolate a unique solution amongst the whole set of possible solutions satisfied by given initial and boundary conditions.

1.2 True and quasi-inhomogeneities

Our attention is concentrated on the wave and front propagation in inhomogeneous media. Material inhomogeneities are theoretically seen as defects in the translational invariance of material properties on the material manifold. Amongst these, we find *true material inhomogeneities*, e.g. material regions of rapid changes in material properties due to a change of constitution; these changes may be more or less smooth or even abrupt. We also find physical and field properties which manifest themselves as *quasi-inhomogeneities* in a general theory of inhomogeneity [Maugin (2003)], i.e. they contribute in the same way as true inhomogeneities to the so-called balance of linear momentum on the material manifold, an equation that just built for that purpose. If the location of rapid changes in material properties due to a change of constitution (true inhomogeneities) is prescribed as initial data, then in contrast quasi-inhomogeneities, such as cracks or phase-transition fronts, are moved during the process and are therefore part of the solution of a particular problem. This is what make this problem simultaneously more interesting and more challenging.

1.3 Driving force and the corresponding dissipation

Here quasi-inhomogeneities provided by field singularities are considered. Unless they have a fractal structure, the support of these singularities may only be zero-, one- or two-dimensional in our three-dimensional physical and material spaces. We focus here on one- and two-dimensional singular sets. As these sets appear to be displaced as a consequence of the general evolution of a field solution under the time-dependent boundary conditions, driving forces acting on them are defined by duality with velocities of points of the sets in agreement with the basic vision of mechanics. The power expended by the driving force should finally be written as the general bilinear form

$$P(\mathbf{f}) = \mathbf{f} \cdot \mathbf{V}, \tag{1.1}$$

where $\mathbf{f}$ is the driving force, and $\mathbf{V}$ is the material velocity of points of the set [Maugin (1993)]. In some cases, the observed motion of singular sets is thermodynamically irreversible, and the force $\mathbf{f}$ of a non-Newtonian nature acquires a physical meaning only through the power (Eq. (1.1)) it expends, as this is, in fact, its definition in a weak mathematical formulation on the material manifold. The irreversible progress of the singularity set is then governed by the second law of thermodynamics. This means (in terms of temperature $\theta_{\mathcal{S}}$ and entropy production $\sigma_{\mathcal{S}}$ at the singularity) that

$$\mathbf{f} \cdot \mathbf{V} = \theta_{\mathcal{S}}\, \sigma_{\mathcal{S}} \geq 0, \tag{1.2}$$

and the closure of the full solution of the evolution problem requires the formulation of a kinetic law relating $\mathbf{f}$ and $\mathbf{V}$ or a hypothesis about entropy production at the singularity. Examples of singular material sets exhibiting a driving force and dissipation are provided by cracks and phase-transition fronts, two examples that will recur in this book.

1.4 Example of a straight brittle crack

Consider a regular (simply connected) material body in which a straight through crack $C(t)$ expands with material velocity V_C at the crack tip (Fig. 1.1). The extension of the crack is collinear to the crack. The crack

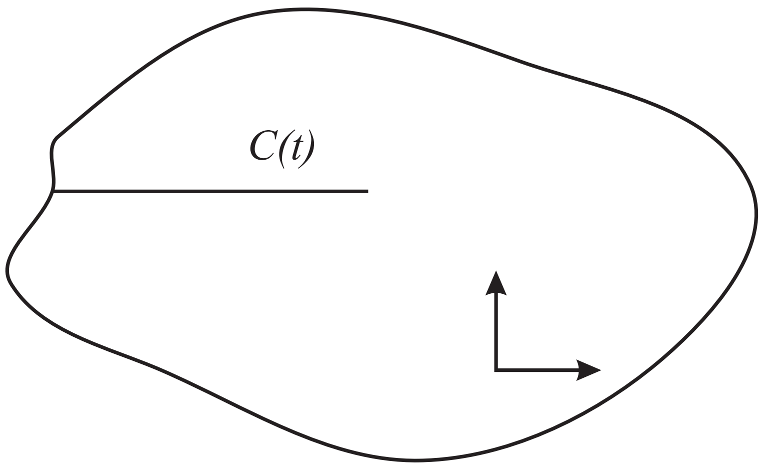

Fig. 1.1 Macroscopic straight-through crack.

tip, in fact, is a straight line but it is seen as a point in a sectional figure drawn orthogonally to this line.

A so-called material force acting at the crack tip (sucking the crack in the body) is none other than the energy-release rate G [Maugin (2000)]

$$G = FV_C = \theta_C\, \sigma_C \geq 0. \tag{1.3}$$

Here the subscript C denotes the crack tip, σ_C is the corresponding entropy production, and θ_C is the temperature at the crack tip.

It should be noted that the energy-release (*time*) rate G may be defined as the decrease of total potential energy Π due to a motion *in a time unit*

$$G = -\frac{\partial \Pi}{\partial t}. \tag{1.4}$$

According to Dascalu and Maugin (1993), this is nothing but the *dissipated power*

$$P_{diss} = G = \mathbf{f} \cdot \mathbf{V} \geq 0, \tag{1.5}$$

where, as in Eq. (1.1), $\mathbf{f}$ is the material driving force, and $\mathbf{V}$ is the material velocity of the crack tip.

Another definition of the energy-release rate (without time involved) is given by (cf. [Ravi-Chandar (2004)])

$$G^* = -\frac{\partial \Pi}{\partial a}, \tag{1.6}$$

where a is homogeneous to a length, e.g., displacement of the crack tip (increase in length) so that Eq. (1.6) is in fact a *material gradient, hence a material force.* Of course one is tempted to write

$$G = G^* \dot{a} = \left(-\frac{\partial \Pi}{\partial a} \right) \dot{a}, \tag{1.7}$$

a result that looks like Eq. (1.5) or Eq. (1.3).

In quasi-statics and in the absence of thermal and intrinsic dissipations, the energy-release rate can be computed by means of the celebrated J-integral of fracture [Rice (1968)] that is known to be path-independent and, therefore, provides a very convenient estimation tool once the field solution is known. However, the velocity at the crack tip remains undetermined and requires additional consideration.

1.5 Example of a phase-transition front

A similar situation holds for a displacive phase-transition front propagation. A stress-induced martensitic phase transformation in a single crystal of a thermoelastic material occurs by the fast propagation of sharp interfaces through the material (Fig. 1.2).

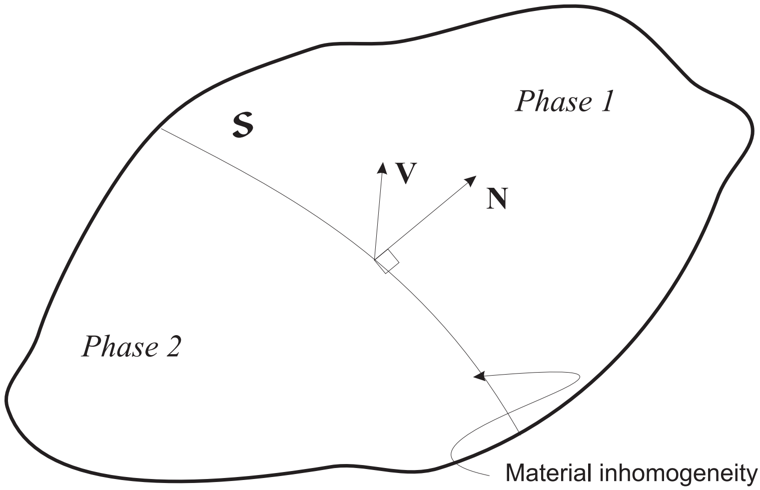

Fig. 1.2 Discontinuity front.

Following the already mentioned balance of pseudomomentum [Maugin (1993)], one can determine the driving force acting on the interface between phases. However, as in the case of the crack tip, this is not enough to determine the velocity of the phase-transition front in crystalline solids. Additional constitutive information is usually provided in the form of a kinetic relation between the driving force and the velocity of the phase boundary. The notion of a kinetic relation is introduced by Abeyaratne and Knowles (1991) following ideas from materials science. It is well understood [Abeyaratne, Bhattacharya and Knowles (2001)] that the kinetic relation is required because of the non-equilibrium character of the phase transformation process. The derivation of the kinetic relation is therefore the main problem in the description of the moving front propagation.

1.6 Numerical simulations of moving discontinuities

To perform numerical simulations of the motion of a discontinuity front we need to know the answers to the following questions in addition to the routine tasks of mesh generation and discretization of governing equations:

- how to compute the value of the driving force acting at the front (and its critical value);
- how to calculate the velocity of the front;

- how to determine the jumps of fields across the discontinuity front.

As we will see, the answers to the formulated questions can be given by a combination of the material formulation of continuum mechanics, the thermodynamics of discrete systems, and finite-volume numerical methods. The description of the corresponding framework and its application is in fact the main subject of the book.

It should be noted that the macroscopic description of moving fronts in solids (such as phase-transition fronts or crack fronts) is based on the conventional local equilibrium approximation (see, e.g. [Freund (1990); Ravi-Chandar (2004)] for cracks and [Abeyaratne and Knowles (2006)] for phase-transition fronts). This means that all the thermodynamic quantities, including temperature and entropy are defined following conventional methods [Callen (1960)]. Extension of the local equilibrium approximation to computational cells of finite volume computational schemes is not really straightforward. First, the local equilibrium values of field variables may be, in general, distinct from their averaged values, as shown by Muschik and Berezovski (2004). Secondly, the numerical fluxes needed for the updating of the local equilibrium state in a computational cell cannot be provided at a moving discontinuity without taking into account the entropy production due to the motion of this discontinuity.

Fortunately, there is a rather nice similarity between the discrete representation of conservation laws [LeVeque (2002a)] and the thermodynamics of discrete systems [Muschik (1993)]. Using this similarity, the Godunov-type numerical schemes for simulation of wave and front propagation can be reformulated in terms of excess quantities [Berezovski and Maugin (2001, 2002)], which appear in the local equilibrium approximation due to the interaction between discrete systems. Moreover, numerical fluxes are determined by means of the non-equilibrium jump relations at moving fronts [Berezovski and Maugin (2005b)], which are also formulated in terms of excess quantities [Berezovski and Maugin (2004)]. The closure of the model is achieved by an assumption concerning the excess quantities behavior across the moving front. This leads to the relation between the stress jump at the discontinuity and the corresponding driving force. Then the velocity of a moving front (the kinetic relation) can be determined [Berezovski and Maugin (2005a)]. As a consequence, we obtain a thermodynamically consistent numerical algorithm which can be applied to both wave and front propagation problems.

1.7 Outline of the book

The whole book is virtually divided into three parts. The first part includes the introduction and three theoretical chapters. In the second chapter, we briefly recall the description of inhomogeneities in the framework of the *material formulation* of continuum mechanics [Maugin (1993); Kienzler and Herrmann (2000)]. The third chapter is devoted to the derivation of non-equilibrium jump relations at discontinuities. The small-strain approximation of balance laws and jump relations used in applications is given in the fourth chapter. The general description of the applied finite volume algorithm is also presented.

In the second part of the book, the developed theory is applied to one-dimensional problems of wave and front propagation. In the fifth chapter, the application of the composite wave-propagation algorithm to the solution of wave propagation problems in media with rapidly-varying properties is demonstrated. The main advantage of the proposed theory is the possibility of its extension to the case of moving boundaries in solids. In this connection, a non-equilibrium description of martensitic phase-transition front propagation in solids is considered in the sixth chapter. The results of numerical simulations of moving phase boundaries in the one-dimensional setting are presented and the comparison with experimental data for impact-induced martensitic phase transition is also given.

Two-dimensional problems are considered in the third part of the book. Wave propagation in heterogeneous solids is the subject of the seventh chapter. Details of the numerical algorithm in two dimensions are also given here. The next chapter is devoted to waves in functionally graded materials. Examples of two-dimensional phase-transition fronts dynamics are considered in the ninth chapter. In the tenth chapter, the dynamics of a straight brittle crack is studied. The velocity of the crack is determined in terms of the driving force by means of non-equilibrium jump relations at the crack front. Numerical simulations are compared with the corresponding experimental data.

Overall conclusions are given in the last chapter. Details of the thermodynamic description in the framework of the thermodynamics of discrete systems are presented in the Appendix.