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# Jog my shape memory—dynamics as a challenge in mathematical materials science

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Many complex phenomena in nature exhibit multiple scales. The challenge is to understand how the effects on one scale influence those on another. This review discusses some aspects of a multiscale analysis of martensitic materials as a prominent example of materials which exhibit nuanced structures and surprising implications on various scales. The emphasis is on dynamic issues. Some speculations are offered on future research directions.

**Keywords:** Phase transitions, martensite, multiscale analysis

## 1. What are martensites?

Everyone has seen phase transitions, i.e., a transformation of a (thermodynamic) system from one phase to another. Melting ice, freezing water or condensing vapour are some classic examples. Less well known, but equally important, are phase transitions occurring between different solid states. Around 1890, the German metallurgist Martens discovered something fairly unexpected, taking advantage of strident progress in optical technology in the 19th century. He inspected steel under a microscope, discovering complex, needle-like structures consisting of different solid phases, which form distinctive patterns, invisible to the naked eye. Two examples are shown in figure 1. Today, such patterns (ranging from a few nanometres to a few microns) are commonly called *microstructures*. The microstructure strongly influences the mechanical properties of the material. For example, the pattern in hard steels is usually more coherent than that in inferior steels.

In honour of Martens' discovery, solid-to-solid phase transitions, where the lattice structure changes abruptly at some critical temperature, are called *martensitic phase transitions*. Obvious questions arising in the context of martensites are: how does the microstructure form? How does it evolve? What is its influence on macroscopic properties? Our understanding of dynamic issues is still in its infancy. In this review article, some recent contributions are outlined, and some future challenges are sketched. To convey the main ideas, we ignore many complicated aspects of real microstructure, preferring to discuss idealised situations. Space limitations oblige us to omit a discussion of many valuable contributions. Fortunately, several excellent surveys offer a rather different emphasis, for example Roubíček (2000) and the monograph by Bhattacharya (2003). Sethna's web-site <http://www.lassp.cornell.edu/sethna/Tweed/> makes for a fascinating read. The state of the art in the passage from quantum chemistry to crystalline (mi-

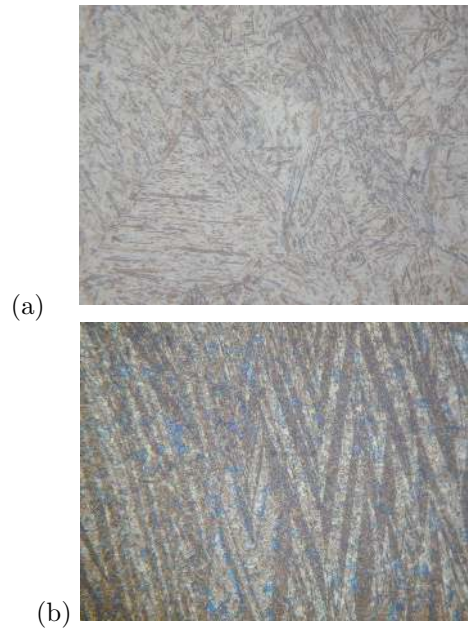


Figure 1. Examples of microstructure in martensitic materials. (a) Reconstructive transformation. The photograph shows martensite in 0.8% carbon steel. (b) Weak transformation. The photograph shows the formation of needles and wedges in NiTi.

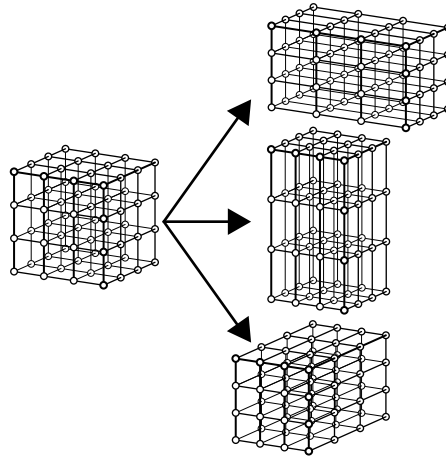


Figure 2. Cubic-to-tetragonal transition. For this transition, the austenitic phase, stable above the critical temperature, is cubic, while the martensitic phase, stable below the critical temperature, is tetragonal. There are three variants of martensite.

oscopic) structures and their macroscopic limits is described by Le Bris & Lions (2005).

The mathematical treatment of microstructured materials dates from the pio-

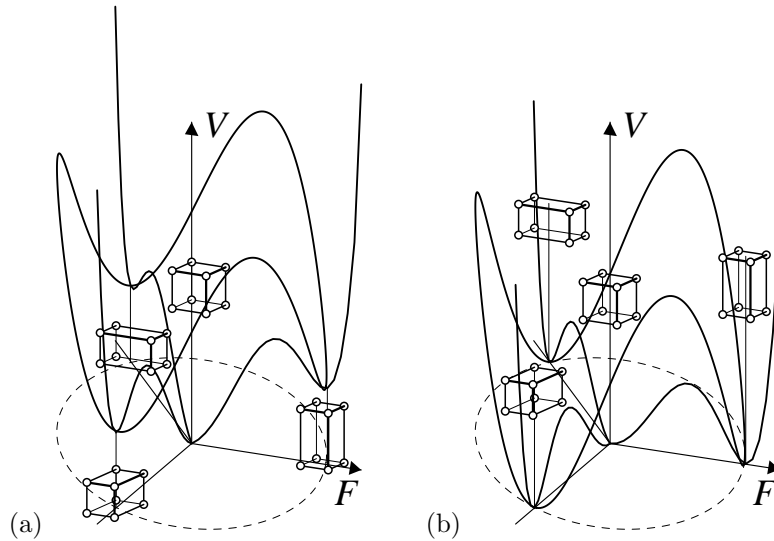


Figure 3. Schematic plot of the energy landscape for the cubic-to-tetragonal transition at different temperatures. The vertical axes represents the density of the potential energy, while the horizontal plane symbolises the different crystalline states (in symmetric coordinates). (a) Above the critical temperature, the cubic lattice is stable, i.e., has the smallest potential energy. (b) At the critical temperature  $\theta_c$ , the austenitic (cubic) and the martensitic (tetragonal) phases are stable.

neering work by Ball & James (1987, 1992), Ericksen (1980) and Chipot & Kinderlehrer (1988). There is an intricate theory based on the concept of global energy minimisation. This has proved highly successful in explaining many phenomena of elastic and plastic behaviour of materials with microstructures. A recent trend is to investigate dynamic aspects, developing a dynamic theory for situations where the material does not attain the ground state (the configuration with the lowest energy). Ball *et al.* (1991) and Friesecke & McLeod (1996) have made early contributions which highlight the importance of dynamical aspects, e.g., by acting as a selection criterion, preventing martensitic materials from forming arbitrarily fine microstructures. For a model proposed by Ball *et al.* (1991), Friesecke & McLeod (1996) study rigorously the dynamics of microstructure formation in a context where energy minimisation predicts the formation of infinitely fine patterns. In experiments, one typically observes pattern formation on a small but finite length scale. This effect can also be seen in the dynamic model (Friesecke & McLeod, 1996). Friesecke & McLeod (1996) prove that for suitable initial data (with strain fields having a transition layer; see §2 for the definition of strain), the limiting patterns for time going to infinity are not global minimisers, but relative ones. Relative minimiser are minimisers in the class of patterns with the same positions for the strain interfaces. One can therefore say that the dynamics selects a relative minimiser, rather than a global minimiser. This highlights a stark contrast between the dynamic and the static picture.

We discuss some recent developments, with the following layout: two different categories of martensitic materials, characterised by weak and reconstructive

transformations, are sketched in §1 (a) respectively §1 (b). Typically, a symmetry breaking occurs for a weak martensitic transformations at the transition point. Phase transformations which are not weak are called reconstructive. In §1, we mention the importance of this classification and some surprising consequences: weak martensitic may exhibit the so-called shape-memory effect (see figure 4); reconstructive phase transformations occur for example in steels and are irreversible. The rest of the paper is dedicated to dynamic aspects of martensitic materials and potential implications beyond martensites. We start the tour in §2 on the continuum scale, which leads to an investigation on the atomistic scale in §3. A discussion of the implication on the continuum scale in §3 (c) completes the cycle. An excursion to dislocation models in §3 (d) shows that similar ideas are applicable in a different context.

(a) *Weak martensitic transformations and the shape memory effect*

What are *weak martensitic transformations*, such as in NiTi? Let us start by inspecting the microstructure and the underlying phase transition, before discussing a surprising implication on the macroscopic scale. An example of microstructure arising in NiTi is shown in figure 1 (b). Weak martensitic transformations are characterised by rapid loss of symmetry of the crystal structure in one direction of the transformation (a slightly more general definition is given by Bhattacharya *et al.* (2004)); they are diffusionless rearrangements of the lattice structure. This is depicted in figure 2 for the cubic-to-tetragonal transition. If no loads are applied, above a critical temperature  $\theta_c$ , the lattice forming the structure is stable in a cubic configuration. Should a temperature drop below  $\theta_c$  occur, three different symmetry-related tetragonal lattices become stable, and the cubic lattice becomes metastable. The high-temperature, high-symmetry phase is commonly referred to as *austenite*, and the low-temperature, low-symmetry phase is called *martensite*. Figure 2 shows that there are three tetragonal *variants* of martensite for the cubic-to-tetragonal transformation.

Suppose a shape memory material is initially in the austenitic state, and we apply an external biaxial load. The material will first deform elastically, as an “ordinary” elastic material. Once a critical load is reached, it will start to transform under stress to martensite. This is called a *stress-induced transformation*. For suitable alignment of the load and the crystallographic axes, one will observe the formation of martensitic twins (due to the coexistence of different variants of martensite at temperatures below the critical temperature). This procedure, called *twinning*, means that atoms on one side of the twin plane undergo a shear displacement relative to the atoms on the other side, in a direction which is parallel to the twin plane. It is often favourable (e.g., to accommodate boundary conditions) to form many interfaces between different martensitic variants. Thus, in this case, twinning occurs on a fine scale, and a microstructure is generated. The formation of twin boundaries obviously increases the interfacial energy, but typically facilitates a very significant reduction of the elastic strain energy of the bulk.

It is not hard to see that the coexistence of several martensitic phases is at the basis of the intriguing shape memory effect, which occurs for example in Nitinol (see figure 4): a deformation can be reversed upon heating. The transformation is

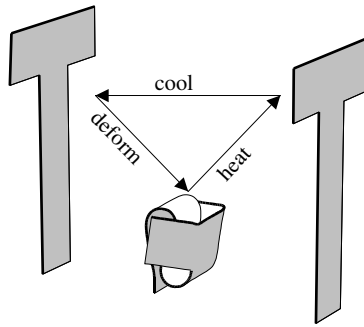


Figure 4. The shape memory effect. Macroscopically, small deformations (depending on the material, typically up to 8%) disappear upon heating the material beyond the critical temperature  $\theta_c$ . When cooling down to temperatures below the critical temperature, the specimen remains macroscopically unchanged.

reversible, and the cycle can be repeated many times. Bhattacharya (2003) offers an excellent discussion of how microstructures give rise to the shape memory effect.

The shape memory effect has numerous applications in medical and engineering devices (Otsuka & Wayman, 1998). These materials are candidates for artificial muscles (de Gennes & Okumura, 2003). Since, always with the shape memory effect in mind, Nitinol enjoys an adaptivity and flexibility ordinary materials are missing, it is regarded as an *adaptive material*. Lessons learnt from the shape memory effect can often be transferred to similar effects occurring in other adaptive materials, such as ferromagnetic shape memory alloys and ferroelectrics. Salje (1993) discusses martensitic phase changes in metals. Olson & Hartman (1982) observe martensitic phase transformations in biological systems, namely the tail sheath of the T4 bacteriophage virus. A relatively sound modelling on the crystalline level makes martensitic materials an ideal sand box for a mathematical analysis of multiscale phenomena. Before discussing mathematical models for the shape memory effect, we first contrast the martensitic transformations in shape memory alloys with those occurring in steels.

#### (b) *Martensites in steel*

Steel is another example of a material forming martensitic structures, and the microstructure plays a decisive rôle in the mechanical properties. Notably, martensitic transformations are induced in steel by quenching (rapid cooling), to enhance the alloy's strength (Olson & Owen, 1992). An ongoing endeavour in casting and rolling of steel products is to influence the microstructure and optimise it in the production process. This industrially relevant problem is not quite fully understood. The challenges are close at hand: steel is usually rolled in mills in order to produce strips of a desired thickness and width. Typically, in a so-called *hot rolling mill*, the strip enters at a speed of 1 m/s at a temperature of 1100°C, and exits at 900°C with a speed of 3–15 m/s. In the subsequent cooling section the strip is cooled down with water to about 500–600°C (M. Kurz and M. Metzger 2006, personal communication). The temperature gradient influences the microstructure, and the

aim is to control a structure, at most, of a few microns at such high speeds and temperatures!

A stark contrast is exhibited between microstructures in steel and shape memory alloys. In the latter, the microstructure formed at low temperature disappears upon reheating, and the transformation is reversible (Otsuka & Wayman, 1998). In the former, a microstructure generated by quenching remains essentially unchanged upon loading or heating, and the transformation is not reversible (Olson & Owen, 1992).

Bhattacharya *et al.* (2004) recently accounted for this difference on the basis of the symmetry of phases involved in the transition. Specifically, they showed that two different classes of martensitic transformations are plausible. One class, which includes steels, sports “cheap” plastic deformations (via lattice-invariant shears) in the sense that such a deformation is energetically not more expensive than a phase transition. The occurrence of plastic deformations then introduces an irreversibility. For the other class, the energetic price for lattice-invariant shears can be much higher than that for phase changes. Consequently, these transformations can be reversible. The common shape memory alloys belong to this class.

## 2. Macroscopic models for shape memory alloys

The question is how to model martensitic materials, and in particular account for dynamic effects in shape memory materials. We begin the journey through mathematical models for shape memory alloys on the macroscopic level, before travelling to the microscopic level, and returning to the continuum (macroscopic world). Though we should pause at the mesoscopic scale to discuss grain boundaries and the polycrystalline nature of materials and their influence on macroscopic properties, we rather refer the reader to the literature (Bhattacharya & Kohn, 1997; Chenchiah & Bhattacharya, 2005; Kružík & Otto, 2004).

Mathematical models for shape memory alloys are often expressed in terms of continuum mechanics. Let us assume that, at a fixed time, the material occupies a region  $\Omega \subset \mathbb{R}^3$ . Then the key variables describing the alloy are the *displacement field*  $u: \Omega \times \mathbb{R} \rightarrow \mathbb{R}^3, (x, t) \mapsto u(x, t)$ , the *velocity*  $\dot{u}(x, t)$ , and the *strain*  $Du = \left( \frac{\partial u_j}{\partial x_k} \right)_{j,k=1,2,3}$ . Let  $\Phi = \Phi(F)$  with  $F \in \mathbb{R}^{3 \times 3}$  denote the elastic energy density, which is a function of the deformation gradient. The (Piola-Kirchhoff) *stress tensor* is  $\sigma(F) = \frac{\partial \Phi(F)}{\partial F}$ .

In classical elastodynamics, the equations of motion are considered as the governing partial differential equations,

$$\rho u_{tt} = \text{Div}(\sigma(Du)) \quad (2.1)$$

(here and in the following, the dynamics are assumed to take place isothermally, since many challenges can already be cast in this setting. The temperature will be below  $\theta_c$ , so that several variants are stable).

### (a) The elastic energy density

A key ingredient to equation (2.1) is the elastic energy density  $\Phi$ , since it determines the stress tensor  $\sigma$ . What is the shape of  $\Phi$  for a shape memory alloy?

This question proves to be surprisingly tricky. In general,  $\Phi = \Phi(F)$ , with  $F$  denoting the deformation, can be written as a function  $\tilde{\Phi}(F^T F)$ , to account for the invariance of the energy under a change of coordinates of an observer. Thus, the energy is a function of the six components of the (right) Cauchy-Green tensor  $F^T F$ . For a martensitic material, the energy has to meet a symmetry condition imposed by the austenitic phase. Symmetric functions in six components with minimisers at prescribed positions, correct elastic moduli (second derivatives) and a phenomenologically correct dependence on the temperature are not easy to write down explicitly.

Consequently, only a handful of specific examples of energy densities can be found in the literature. A prominent one is given by James (unpublished notes, 1988) and Ericksen (1986) for the cubic-to-tetragonal transformation in InTi. Vedantam (2000) uses irreducible polynomials of the strain tensor to derive an elastic energy density for CuAlNi. A different line of thought introduces symmetry-adapted non-linear coordinates in conjunction with suitable splines (Zimmer, 2004; Hormann & Zimmer, 2006); the additional degrees of freedom make it possible to fit elastic moduli which cannot be fitted with invariant polynomials of lowest order.

There seems to be no general framework to derive macroscopic energy densities from *ab initio* calculations. However, Vedantam (2000) specialises his macroscopic energy density to a shear deformation on a twin plane along the twinning direction and obtains a remarkable agreement with an energy calculated from molecular statistics. The approach to combine symmetry-adapted coordinates and splines may provide a general method to accommodate the wealth of data obtained by *ab initio* calculations.

### (b) *Ill-posed equations of motion*

Unfortunately, the problems only start once we have chosen an energy density and try to solve an initial-boundary value problem for (2.1). To see this, let us consider the simplest situation, a one-dimensional bar under a tensile force. We also ignore effects of inertia and consider the equilibrium situation. It is not hard to see that the equilibrium configuration is generically not uniquely determined; any of the infinitely many solutions involving a mixture of stable variants may be the material's response to the applied force.

It is useful to reformulate this insight in mathematical terms. Since  $\Phi$  is nonconvex for low temperatures, the stress tensor will be non-monotone. It is immediate that the hyperbolicity condition  $\sigma'(u_x) > 0$  is thus violated. This implies that equation (2.1) changes type.

Young measures have been introduced as generalised solutions (Ball & James, 1987). For details we refer the reader to lecture notes by Müller (1999).

### (c) *Rankine-Hugoniot conditions*

The ill-posedness of (2.1) arises as a consequence of the coexistence of two phases. Thus, let us investigate the situation more closely at an interface between two coexistent phases. For simplicity, we think of the interface as straight. It is convenient to take unstressed austenite as the reference configuration; then two martensitic variants meeting at the interface are generated by different deformations, since



they are characterised by a distinct crystallographic lattice and orientation. Thus, at the interface, the strain will be discontinuous.

This simple observation is already the key, as becomes apparent once we apply a force in this *Gedankenexperiment* to “jog the shape memory”, i.e., make the phase boundary move. Assume the force favours one of the two variants at the interface. Then the interface propagates towards the phase with higher energy, since this is transformed into the low-energy phase. It is not hard to see that a discontinuity such as the interface cannot move arbitrarily; the *Rankine-Hugoniot* conditions state that, if the interface moves with the velocity  $\dot{s}$  and either the strain  $u_x$  or the velocity  $\dot{u}$  are discontinuous at the interface, the following relations must hold:

$$\begin{aligned} \llbracket \sigma(u_x) \rrbracket &= -\rho \llbracket \dot{u} \rrbracket \dot{s}, \\ \llbracket u_x \rrbracket \dot{s} &= -\llbracket \dot{u} \rrbracket, \end{aligned}$$

where, for a function  $f(x, t)$ ,  $\llbracket f \rrbracket$  stands for  $f(s(t)+, t) - f(s(t)-, t)$ , i.e., the difference of the limiting values from the right and from the left.

A moving interface can be seen to dissipate energy, and the amount of dissipation is measured by the *configurational force* (or *driving force*). To define it, we let  $\{\sigma\} := \frac{1}{2}(\sigma(s(t)+, t) + \sigma(s(t)-, t))$  denote the average stress across the discontinuity. Then, the configurational force is

$$f := \llbracket \Phi \rrbracket - \{\sigma\} \llbracket u_x \rrbracket.$$

The rate of the energy dissipation is then given by  $f\dot{s}$ . The entropy inequality requires that  $f\dot{s} \geq 0$ .

There are two kinds of moving interfaces, subsonic or supersonic with respect to the sound speed of the surrounding elastic medium, which is here the same for both phases. Supersonic phase boundaries satisfy the Lax condition for hyperbolic PDEs, while subsonic phase boundaries violate this condition, and it can be seen that this leads to an ill-posed initial problem for (2.1). Thus, unless otherwise indicated, we focus on the subsonic case, since it poses particular challenges.

For subsonic waves, how can physically relevant solutions be singled out to make the problem well-posed? Abeyaratne & Knowles (1991) introduce a *kinetic relation* as additional constitutive information to determine the macroscopic response of the body. The kinetic relation determines a functional dependence of the configurational force on a phase boundary and a velocity:

$$f = f(\dot{s}).$$

The motivation behind this line of thought is that, according to the principles of irreversible thermodynamics, the propagation speed of the interface is determined by the configurational force, even though the laws of thermodynamics only impose restrictions on this relationship without specifying the relationship explicitly (Abeyaratne & Vedantam, 2003).

(d) *Which kinetic relation?*

It is not obvious how to derive kinetic relations, and different approaches have been taken.



Figure 5. The model of discrete elasticity considered in §3. The atoms are coupled to their neighbours by nonlinear springs.

One approach is to augment equation (2.1) by regularising terms and derive kinetic relations from the augmented model. This is a successful strategy, but the physical meaning of the regularisation is not immediate in the case of shape memory alloys. The complex nature of martensitic phase transitions, exhibiting a very rich phenomenology on various scales, casts some doubts on the possibility of choosing a regularisation on physical grounds, be it by a penalisation of interfaces (capillarity) or by artificial viscosity.

Alternatively, it is not unreasonable to model kinetic relations phenomenologically. Abeyaratne & Knowles (1997) calculated kinetic relations for an austenite-martensite interface in CuAlNi and found dry-friction type of behaviour.

Here, a different line of thinking is presented. The key idea is to resort to the atomistic level. Namely, underlying the macroscopic kinetic relation is the dynamics of the lattice as a result of the crystallographic transformation of one variant into another. Thus, let us replace equation (2.1) with a discretized counterpart. We obtain a model of discrete elasticity, where a one-dimensional body is simply regarded as a chain of atoms, linked by springs which represent chemical bonds. Lattice models automatically generate a kinetic relation as a consequence of radiative damping (Kevrekidis & Weinstein, 2000).

### 3. Lattice models

We consider a two-sided infinite chain of atoms, and assume nearest neighbour interactions, see figure 5. The atoms are identical and, in normalised variables considered below, they have unit mass. The springs are identical, but will be nonlinear. For each spring, the elastic energy is a function  $\Phi: \mathbb{R} \rightarrow \mathbb{R}$ , which takes the discrete strain as the argument.

The scaling is such that the reference interparticle distance is one. For atom  $k \in \mathbb{Z}$ , the displacement is  $u_k: \mathbb{R} \rightarrow \mathbb{R}$ . The discrete strain is given by the difference of the displacements,  $u_{k+1}(t) - u_k(t)$ , say. Newton's law then gives the equations of motion,

$$\ddot{u}_k(t) = \Phi'(u_{k+1}(t) - u_k(t)) - \Phi'(u_k(t) - u_{k-1}(t)) \quad (3.1)$$

for every  $k \in \mathbb{Z}$ .

#### (a) A fifty-year old challenge: anharmonic interaction potential

The study of equation (3.1) has a lively history, which can be traced back at least to a famous computer experiment by Fermi *et al.* (1955) in Los Alamos. They considered a chain of 64 identical atoms, interacting with their nearest neighbours as described by (3.1), with an anharmonic potential  $\Phi$ , with a sinusoidal initial condition. The anticipation was that equipartition of the energy would occur, meaning that the lattice would reach a thermal equilibrium, and that averaged over time, the initial energy would be equipartitioned among all Fourier modes. Astonishingly,

the discovery was that the system did not approach thermal equilibrium, but behaved essentially quasi-periodically; thermalisation was only found for an initial energy exceeding a certain threshold. Significant progress has been made in the mathematical analysis of the Fermi-Pasta-Ulam (FPU) lattice. Friesecke & Wattis (1994) use a variational approach to obtain localised solutions, and Friesecke & Pego (1999) give in a series of impressive papers a very detailed description of solitary waves in the FPU lattice. Iooss (2000) uses a centre manifold approach to find all small bounded travelling waves for generic elastic energies near the first critical wave velocity. These results either assume the convexity of the elastic energy, or prove results for small amplitude solutions, where it is an open question whether the confinement to a convex region within the potential can be overcome.

(b) *Travelling phase transitions on the atomistic scale*

For phase transitions,  $\Phi$  is nonconvex and thus the springs are bistable. This nonconvexity makes the mathematical analysis even harder, and our current understanding of this situation is very fragmentary.

To identify the kinetic relation, it is natural to seek travelling waves as solutions to equation (3.1). A travelling wave is a special solution of the form

$$u_k(\xi) := u(k - ct). \quad (3.2)$$

We insert this ansatz in equation (3.1) and obtain

$$c^2 \ddot{u}(\xi) = \Phi'(u(\xi + 1) - u(\xi)) - \Phi'(u(\xi) - u(\xi - 1)). \quad (3.3)$$

Does equation (3.3) have a solution? Truskinovsky & Vainchtein (2005) consider the case where the elastic energy is piecewise quadratic (and each particle may interact with  $l$  neighbours, with a quadratic energy for every interaction except for the nearest neighbours). An explicit solution can be computed which has a vanishing strain at 0 and two different strains as  $\xi \rightarrow \pm\infty$ ; the atoms at the left of the interface are in one phase, while those on the right are in the other phase.

For a general elastic energy, the picture is largely open. Schwetlick & Zimmer (2006) prove the existence of *supersonic* solitary waves, where the strain is asymptotically for  $\xi \rightarrow \pm\infty$  in one state (the left well of the elastic energy, say), and in between makes an excursion towards the right well. The proof relies on a mountain pass argument and assumes a sufficiently high wave speed  $c$ . A qualitative description of the solution is not known. In particular, it remains open whether the homoclinic excursion in the strains reaches the second well. Another challenging open problem concerns the stability of these solitary waves.

(c) *Return journey to the macroscopic world*

For a piecewise linear stress-strain relation, specifically for a nearest-neighbour interaction potential which is the pointwise minimum of two quadratic wells, one can compute more, and use the microscopic information on the journey back to the macroscopic world. We recall that the microscopic model (3.1) is Hamiltonian, but the kinetic relation is to specify a macroscopic dissipation. Truskinovsky & Vainchtein (2005) construct explicit (microscopic) travelling wave solutions (with piecewise quadratic interaction potential) and show that the radiation of lattice

waves carrying energy away from the propagating front results in a macroscopic dissipation. There seems to be no rigorous proof of stability for the travelling waves, but numerical simulations (Truskinovsky & Vainchtein, 2005) indicate that at least some of the travelling waves are stable. For the same setting, Truskinovsky & Vainchtein (2006) give various dispersive quasicontinuum approximations, based either on Taylor or rational (Padé) approximations, and show that the associated kinetic relation agrees well with its microscopic prediction.

Abeyaratne & Vedantam (2003) derive a kinetic relation for twin boundary motion from a lattice model. They consider a ledge propagating transversely along the twin boundary. Abeyaratne & Vedantam (2003) determine the forward motion of the twin, and pass to the continuum using a higher order expansion. The lattice model resembles the Frenkel-Kontorova model discussed in (d) below. Remarkably, in the continuum limit, the solution exhibits an oscillatory behaviour behind the travelling wave, rather than converging asymptotically to a fixed displacement.

(d) *An excursion to dislocations*

The analysis of travelling waves and kinetic relations for phase transitions bears many similarities with the analogous study of dislocation dynamics. A simple model of the latter has been given by Frenkel and Kontorova in 1938. The governing equation is

$$\ddot{u}_k(t) = \gamma (u_{k+1}(t) - 2u_k(t) + u_{k-1}(t)) - V'(u_k(t)), \quad (3.4)$$

which differs from equation (3.1) in the sense that the elastic energy is here assumed to be harmonic, and there is an additional *on-site potential*  $V$ . For the Frenkel-Kontorova model,  $V$  is periodic,  $V(u) = -\cos(u)$ . Again,  $u_k$  denotes the displacement of particle  $k$ ; the coupling constant  $\gamma$  is strictly positive.

In the mathematics literature, (3.4) is often referred to as the *discrete Klein-Gordon equation*. Then,  $V$  is taken to be anharmonic and analytic with  $V(0) = 0$  and  $V''(0) > 0$ . Here, the centre-manifold approach yields “nanopterons” (solitary waves superposed on exponentially small oscillatory tails), as shown by Iooss & Kirchgässner (2000). Of particular interest here are *travelling breathers*, i.e., spatially localised solutions which are time-periodic in a system of reference moving at constant velocity. Numerical calculations here as for the Fermi-Pasta-Ulam chain are a delicate task. Duncan *et al.* (1993) report that they could only find travelling waves superposed to a tail which appears periodic with a small amplitude, but no travelling waves with the property  $u(z) \rightarrow 0 \pmod{2\pi}$  as  $z \rightarrow \pm\infty$ . It may be that this background radiation is necessary to enable a lossless propagation of the wave. Likewise, it is possible that the exponentially small tails are essential for the propagation of a wave which is otherwise solitary. This phenomenon seems not to be understood.

Currently, there is no rigorous framework for the passage from the atomistic scale to the continuum for dislocation dynamics. Carpio *et al.* (2001) discuss some continuum models for dislocation densities and highlight open problems. Again, some models are ill-posed, and thus some challenges resemble those we discussed earlier for martensites. The forthcoming book by Cai and Bulatov (W. Cai and V. Bulatov, *Computer Simulations of Dislocations*) offers a detailed discussion of dislocation dynamics on different scales.

(e) *Modulation and macroscopic models*

Modulation theory gives a formal way of deriving a thermodynamic description for lattice models. Here, the goal is to obtain macroscopic equations describing temperature effects due to microscopic oscillations, rather than to find kinetic relations. We thus leave the world of phase transitions and dislocations and consider lattice models with convex interaction potentials. Let us assume that the microscopic dynamics is described by equation (3.1) (thus,  $t$  is the *microscopic time* and  $k$  is the *microscopic particle index*). From this information, we would like to infer the evolution of macroscopic thermodynamic fields, such as momentum, energy and entropy.

A powerful, yet formal procedure for this micro-macro transition is as follows. On the microscopic level, temperature corresponds to oscillatory behaviour of the atoms. Thus, it is reasonable to consider periodic travelling waves which may mimic these oscillations. Let the travelling wave be given as  $u_k(t) = rk + vt + u(jk + \omega t)$  for  $k \in \mathbb{Z}$  (compare (3.2)). The parameters are: mean distance  $r$ , mean velocity  $v$ , wave number  $j$  and frequency  $\omega$ . We define a *macroscopic time*  $\tau := \epsilon t$  and a *macroscopic particle index*  $y := \epsilon k$  (this the *hyperbolic scaling*; other scalings yield the Korteweg-deVries equation (Friesecke & Pego, 1999) and the nonlinear Schrödinger equation (Giannoulis & Mielke, 2006) as governing macroscopic evolution equations). The main idea of modulation theory is to consider approximate travelling wave solutions by allowing the travelling wave parameter to vary on the macroscopic scale. The travelling wave parameters become fields in the macroscopic variables  $\tau$  and  $y$ . Dreyer *et al.* (2006) describe this procedure and obtain four conservation laws for the four parameters  $r$ ,  $v$ ,  $j$  and  $\omega$ , known as Whitham's equations. We refer the reader to the literature (Dreyer *et al.*, 2006) for the precise procedure and further references.

Giannoulis & Mielke (2006) proved the validity of the nonlinear Schrödinger equation as an approximation of a nonlinear version of the Klein-Gordon equation (where the interaction potential is allowed to be nonlinear) with a nonlinear on-site potential for large, but finite time intervals. For the Fermi-Pasta-Ulam lattice, the validation of a modulation equation seems to be open.

## 4. Looking ahead

Several open problems for martensitic materials have been highlighted in the previous discussion, and they are challenging mathematical questions in their own right. On the atomistic scale, key challenges are to remove a smallness assumption, for example on the amplitude of a wave, and thus gain a qualitative knowledge of lattice waves in phase-transforming materials. Furthermore, the rigorous passage from atomistic to continuum is widely open.

Implications of a deeper mathematical appreciation are likely to go beyond shape memory alloys. In general, our understanding of the micro-macro transition is very poor. For example, does the motion of defects give rise to friction, a phenomenon we encounter every day but do not understand well at all? If so, can we develop mathematical ways of deriving macroscopic descriptions for, say, defect densities and their motion, rather than postulating such laws phenomenologically?

There are other examples of defect dynamics which we would like to understand better, among them crack tips, and interstitials and vacancies. Defect phenomena on the atomistic scale are of direct relevance to materials science, solid state physics, and physical chemistry. For many applications, such as fuel cells, these transport phenomena need to be understood. The movement of a martensitic phase boundary may be seen as a relatively simple problem with a moving singularity, and further advancement in this field is likely to spark insights in the aforementioned disciplines.

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