Dynamics of patterns in ferroelastic-martensitic transformations. I. Lattice model

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(Received 20 February 1990; revised manuscript received 25 July 1990)

A lattice model and its nonlinear dynamics for ferroelastic-martensitic transformations is proposed. The lattice model presented involves the necessary interactions required in a cubic-tetragonal transformation for proper ferroelastic materials for which the strain tensor is merely the order parameter. Basically, the lattice model is a two-dimensional system including both nonlinear and competing interactions. The latter are considered as two kinds: (i) interactions by particle pairs and (ii) noncentral interactions or bending forces. A one-dimensional version is derived from the two-dimensional system, with the former possessing the anisotropic nature of the original lattice. The equations of motion are deduced as a set of difference-differential equations placing thus the discrete macroscopic and microscopic stresses in evidence. Moreover, upon investigating homogeneous states of deformation of the lattice, a comparison can be made with the Landau theory for ferroelastic phase transitions. On the basis of this reduced one-dimensional model the softening of the transverse-acoustic-phonon branch is examined, leading to two important results: (i) the partial softening of this branch of dispersion at a nonzero wave number and (ii) the positive curvature of the dispersion curve at the long-wavelength limit. All these effects are usually observed by means of neutron-inelastic-scattering techniques and this suggests pretransitional effects characterized by modulated lattice distortions.

I. INTRODUCTION

The goal of the present study is to examine the *nonlinear dynamics of microstructure patterns* made of elastic domains involved in *ferroelastic-martensitic transformations.* Our main purpose is the understanding of the underlying microphysics which induces special kinds of strain transformations associated with the elastic domain formation. With this in mind, we consider a reduced one-dimensional model extracted from a real two-dimensional lattice model and its continuum approximation. The paper is devoted especially to the microscopic model and the phonon dispersion associated with the lattice vibration, whereas the quasicontinuum model and nonlinear excitation solutions will be proposed in the companion paper. From the physical point of view, within the overall class of displacive diffusionless phase transformations, martensitic transformations are characterized by involving lattice distortion and shear displacements.[1,2] That means the transformation is mostly dominated by strain energy. As a consequence, the transition is of *first order,* where the spontaneous strain is the order parameter in the Landau theory of phase transition and the ferroelasticity is called proper.[2,3] For instance, In-Tl, Ni-Ti, Fe-Pd, and others are good candidates of such alloys. Crystals undergoing such transformations exhibit particularly interesting effects: *elasticity, pseudoelasticity,* and *ferroelasticity,* which are intimately connected with phase-transition phenomena as well as *shape-memory effects* of which the technological applications are especially promising. All these effects are only observed at the scale of the crystalline specimen. On the other hand, the continuum thermodynamics approach of such transformations is often built by introducing internal variables which characterize the percentage of austenite and martensitic variants in the crystal.[4] Moreover, these effects are particularly monitored by the dynamics and formation of twin interfaces (walls) and twin bands which are a common occurrence in structural and martensitic phase transitions. As a consequence of the first-order phase transition, the symmetry of the low-temperature phase or the *parent* (untransformed) phase allows for forming a few distinct *variants* or *twins* of the product (transformed, i.e., lattice distortion) phase.[2] Moreover, an external stress causes the twin boundaries to move in order to accommodate the internal stresses. However, stress release results in a return of boundaries to their original positions, which may explain the memory effect. The twin formation and nucleation are usually observed by means of electron microscopy[5,6] and the morphology of the martensitic twinning (deformed lattice) seems to be very rich and interesting.

In the present study we focus on ferroelastic-martensitic transformations and examine an intrinsic mechanism of the elastic twin formation as well as their dynamics. A nucleation process can be seen as a pretransitional modulated structure developing in the high-temperature or parent phase which thus forms a periodically modulated array of parallel twin bands. The latter can be incommensurate with the parent phase.[7–9] It follows, therefore, that coherent motions of twin boundaries are of great importance in understanding the transformation. Indeed, upon cooling a single crystal of austenite, different martensite variants are induced and the application of a stress gives rise to interfacial movements which lead to a macroscopic permanent strain. Upon heating towards the high-temperature phase, the initial single crystal is recovered and initial shape, too. We point out

the interest of the lattice model, because the latter possesses the underlying physical ingredients which are the basis of the phenomena. Many macroscopic properties of materials, mechanical responses to external stimuli for instance, are often the homogeneous result of complex structures or microscopic textures occurring in materials. These microstructures are well described at an *intermediate scale* where the background microscopic scale provides *competing* or *cooperative interactions* and strongly *nonlinear lattice potentials* giving rise to *nonlinear coherent* and *complex structures.*

Many works both experimental and theoretical have been devoted to martensitic transformations and a variety of models have been considered. The traditional metallurgist's point of view usually introduces the dislocation concept[10] to explain the growth mechanism related to a critical size of martensitic embryos. Some microscopic models have been examined for martensitic twinning and are devoted to acoustic-phonon softening and the stability of lattice structures.[11–13] However, special attention is paid to the work of Barsch and Krumhansl[14,15] and Mazor and Bishop,[16] who have developed a general model from the continuum mechanics point of view in order to describe the structure of twin boundaries in cubic-tetragonal ferroelastic transformations as kink-type solitary waves. In the second part of this work, a quasicontinuum model will be presented in this spirit and twin boundaries will be examined.

We focus our attention on a lattice model which enables us to describe a cubic-tetragonal transformation; for instance, the In-Tl or Fe-Pd crystal undergoing a ferroelastic transition of the first order has fcc ($m3m$) symmetry above the transition point and fct ($4/mmm$) below.[17,18] Based on a complete two-dimensional lattice easily extended to a three-dimensional system, we consider the following types of interactions between particles: (i) interactions by *particle pairs* between the first-nearest neighbors and (ii) interactions of the *three-body type* (between three adjacent particles) or noncentral interactions. In addition, the lattice *anisotropy* which derives from the dimensionality of the model allows us to place the predominance of the $[1\bar{1}0]$ direction in evidence. In a cubic-tetragonal transformation $[1\bar{1}0]$ is the direction of the close-packed atomic planes stacked in the [110] direction. Because of the anisotropy and of course of the special type of interactions, the material then exhibits anomalously low anisotropy *shear modulus softening* (transverse-acoustic branch in the [110] direction) which is strongly temperature dependent; nevertheless, the mode softening never takes place completely because of the first-order transition.[19–22] Structural modulations can develop within the parent phase with periodic deformation patterns of which the wavelength corresponds to that of phonon anomalies.[7,23,24] The origin of such patterns can emerge from competing interactions (accounting for the nearest-neighbor and noncentral interactions). Accordingly, a rather fine scale of lattice description seems to be necessary.

The paper is organized as follows. Section II is devoted to the construction of the lattice model itself. Starting with a complete two-dimensional system, particular interatomic interactions are introduced: (i) interactions between next-nearest neighbors and (ii) interactions describing noncentral forces. Although we begin with a two-dimensional lattice model, which is essential to introduce the correct interactions, the one-dimensional version, derived in Sec. III, enables us to describe the shearing motion of the close-packed atomic planes $(1\bar{1}0)$ in the [110] direction. The equations of motion for the microscopic model are deduced from the Hamiltonian of the one-dimensional system in Sec. IV. A comparison with the Landau theory of phase transition is made next in Sec. V for homogeneous states of deformation. The dispersion of transverse-acoustic phonons is examined in Sec. VI, which reveals the softening of the shear mode propagating in [110] with polarization in $[1\bar{1}0]$ related to the martensitic transformation. By way of conclusion, the quasicontinuum model, which will be tackled in the following paper, is finally evoked.

II. CONSTRUCTION OF THE LATTICE MODEL

A. Geometrical considerations

Let us consider an atomic plane extracted from a cubic lattice, such as the fcc symmetry of In-Tl (undeformed state). Nevertheless we assume that the deformation of the lattice along a perpendicular direction to the atomic plane, say the [001] direction, is homogeneous, which means that we deal with plane deformation in the (001) plane. The *geometry* of the lattice plane, in its undeformed state, is made of squares parallel to the [100] and [010] crystallographic directions (see Fig. 1). A particle of the plane is then located by (i,j) in the coordinate system $\{[100], [010]\}$ or $(\mathbf{i},\mathbf{j})$ or by (I,J), in $\{[110], [1\bar{1}0]\}$ or $(\mathbf{I},\mathbf{J})$ deduced from the former by a rotation 45° clockwise. Then, the absolute position of a particle of the un-

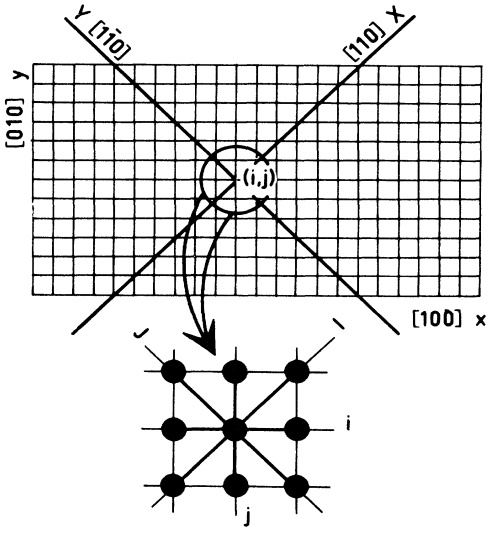

FIG. 1. Geometry of the lattice model: two-dimensional system made of squares. Interactions of the particle at (i,j) with the first-nearest neighbors.

deformed lattice at (i,j) is given by

$$\mathbf{X}(i,j)=(ia)\mathbf{i}+(ja)\mathbf{j} , \tag{1}$$

where a denotes the lattice spacing. After deformation of the lattice the same particle takes on the new position

$$\mathbf{x}(i,j)=\mathbf{X}(i,j)+u(i,j)\mathbf{i}+v(i,j)\mathbf{j} , \tag{2}$$

where $u(i,j)$ and $v(i,j)$ are the longitudinal and transverse displacements, respectively. Since the coordinate system (I,J) can be useful for further developments, the corresponding displacements in the system $(\mathbf{I},\mathbf{J})$ are

$$\begin{aligned} U(I,J)&=[u(i,j)+v(i,j)]/\sqrt{2} , \\ V(I,J)&=[u(i,j)-v(i,j)]/\sqrt{2} , \end{aligned} \tag{3}$$

and we have the associated indexes

$$I=i+j, \quad J=j-i . \tag{4}$$

Accordingly, the position of any particle in the deformed lattice is in the system $(\mathbf{I},\mathbf{J})$,

$$\mathbf{x}(I,J)=[Ib+U(I,J)]\mathbf{I}+[Jb+V(I,J)]\mathbf{J} , \tag{5}$$

where now $b=a/\sqrt{2}$ is the lattice spacing between atomic planes along the directions [110] and $[1\bar{1}0]$. In particular, if the problem concerns only the relative shearing displacements of atomic planes $(1\bar{1}0)$ stacked in the direction [110], we will choose the second coordinate system.

B. Interatomic potentials

We define the interatomic forces acting on the particles of our lattice next. We assume that the particle at the site (i,j) interacts with the first-nearest neighbors surrounding it. We first consider the interatomic interactions leading to potentials which are functions of *particle pairs* between the nearest particles in the four directions $\mathbf{i},\mathbf{j},\mathbf{I},\mathbf{J}$. We consider next a second kind of interaction acting on particles as *noncentral forces* (or three-body interactions), which is equivalent to bond bending or torsional forces and involves three center forces due to the long range of electronic covalent atomic interactions.[25,26] The lattice potential must then account for the change in angle between bond segments joining particle pairs. These interactions describe, at the microscopic level, the twisting and bending of the unit crystalline cell.[27] Roughly speaking, we can say that they are equivalent, in some sense, to the interactions between first neighboring "elastic dipoles" since these interactions include differences of the discrete deformations themselves. Since the lattice energy must be translationally and rotationally invariant, it depends only on the modulus of the relative lattice positions. In fact, after some algebraic manipulations we are able to show that the lattice energy must be a function of the discrete Lagrangian deformation tensor including geometric nonlinearities and also a function of the first-order finite differences of those discrete deformations. Furthermore, it is noteworthy, by dropping the discrete functions, that the discrete description is somewhat similar to that of continuum mechanics[28,29] involving weakly nonlocal behavior or strain gradient elasticity.

III. ONE-DIMENSIONAL MODEL

Because we are interested in the one-dimensional problem here, we assume that the lattice displacements depend only on the I index. With the use of the coordinate system (I,J) and the displacements U and V along the [110] and $[1\bar{1}0]$ directions [see Eq. (3)], respectively (or the I and J directions), we can prove first that the dilational part of the deformation is zero, which, in turn, implies that

$$U(I)=U_0=\text{const} . \tag{6}$$

Equation (6) means that the lattice deformation along the I direction is homogeneous. Second, the lattice deformation is now described by the relative shear deformation along the $[1\bar{1}0]$ direction given by

$$s_I=[V(I+1)-V(I)]/a . \tag{7}$$

Under these hypotheses and by using the deformation (7), the lattice potential of the two-dimensional system can be written as

$$\begin{aligned} \mathcal{V}=\sum_I (&\varphi_1[a(1+\sqrt{2}s_I+s_I^2)^{1/2}]+\varphi_2[a(1-\sqrt{2}s_I+s_I^2)^{1/2}]+\varphi_3\{\sqrt{2}a[1-\tfrac{1}{2}(s_{I+1}+s_I)^2]^{1/2}\} \\ &+\psi_1(a|s_I-s_{I-1}|)+\psi_2(a|s_I+s_{I+1}-s_{I-1}-s_{I-2}|)) . \end{aligned} \tag{8}$$

The potentials φ_α $(\alpha=1,2,3)$ are functions of particle pairs between the first- and second-nearest neighbors in the [100], [010], and [110] directions, respectively. The potential ψ_1 emerges from the noncentral interactions in both [100] and [010] directions and the potential ψ_2 is due to the action of the noncentral forces in the [110] direction. We note that the lattice potential (8) does not depend on the $[1\bar{1}0]$ direction since the lattice motion is homogeneous in the J direction. Now the next step consists of expanding the interatomic potentials with respect to the discrete strains up to the fourth order and second order in their first-order finite differences, to yield

$$\begin{aligned} \mathcal{V}-\mathcal{V}_0=\sum_I [&\tfrac{1}{2}a_1 s_I^2-\tfrac{1}{3}a_2 s_I^3+\tfrac{1}{4}a_3 s_I^4+\tfrac{1}{2}c_1(s_{I+1}+s_I)^2 \\ &+\tfrac{1}{2}d_1(s_I-s_{I-1})^2 \\ &+\tfrac{1}{2}d_2(s_I+s_{I+1}-s_{I-1}-s_{I-2})^2] . \end{aligned} \tag{9}$$

In the expansion (9) the coefficient a_1, a_2, a_3, c_1, d_1, and d_2 are connected with the potential derivatives through

the relations

$$a_1=\frac{a^2}{2}(\varphi_1''+\varphi_2'')\ , \tag{10a}$$

$$a_2=-\frac{3a^2}{8}\sqrt{2}\left[\varphi_1''-\varphi_2''+\frac{a}{3}(\varphi_1'''-\varphi_2''')\right]\ , \tag{10b}$$

$$a_3=\frac{a^2}{8}\left[-\varphi_1''-\varphi_2''+2a(\varphi_1'''+\varphi_2''')+\frac{a^2}{3}(\varphi_1^{(4)}+\varphi_2^{(4)})\right]\ , \tag{10c}$$

$$c_1=-a\sqrt{2}\varphi_3'(2\sqrt{2}a)\ , \tag{10d}$$

$$d_1=a^2(\psi_1''+\psi_2'')\ , \tag{10e}$$

$$d_2=a^2\psi_3''\ , \tag{10f}$$

where all the derivatives are defined at the equilibrium of the lattice, that is when all s_I are zero. So that $\varphi_1'=\varphi_2'=0$, $\psi_1'(0)=\psi_2'(0)=\psi_3'(0)=0$ but $\varphi_3'\neq 0$. Note that we have not specified the form of the interatomic potential and the model is then valid for all sorts of potential. Now, the physical meaning of each term of (9) can be explained. The first three terms of (9) are derived from the nonlinear interatomic potentials between next-nearest neighbors, including a cubic term. The fourth term of (9) describes the interaction between second-nearest neighbors and the last two terms emerge from the three-body interactions between first- and second-nearest neighbors. The lattice deformation is now well described by s_I which represents the *relative shear displacement* of the close-packed atomic planes $(1\bar{1}0)$ in the stacking direction [110]. It is noteworthy that the original two-dimensional lattice model which involved only interactions between first-nearest neighbors leads to a reduced one-dimensional lattice model accounting for interactions between first- and second-nearest neighbors. This means that even if we deal with a one-dimensional lattice, it is worthwhile starting from a complete two-dimensional lattice. We notice that the cubic term which plays an important role in the phase-transition process is derived from the anisotropy of the lattice, even in the one-dimensional version. Indeed, the lattice anisotropy implies $\varphi_1'''\neq\varphi_2'''$ yielding $a_2\neq 0$. We add to the interatomic potential (9) the kinetic energy associated with the transverse displacement $v(I)$

$$K=\sum_I \tfrac{1}{2}M\dot{v}^2(I)\ , \tag{11}$$

where M holds for the mass of any particle of the $(1\bar{1}0)$ plane. The Lagrangian of the system can now be rewritten as (in dimensionless notations)

$$\mathcal{L}=\sum_I \tfrac{1}{2}\dot{V}^2(I)-\sum_I\{\tfrac{1}{2}\alpha S^2(I)-\tfrac{1}{3}S^3(I)+\tfrac{1}{4}S^4(I)+\tfrac{1}{2}\beta[S(I+1)+S(I)]^2+\tfrac{1}{2}\delta[S(I)-S(I-1)]^2$$
$$+\tfrac{1}{2}\eta[S(I+1)+S(I)-S(I-1)-S(I-2)]^2\}\ , \tag{12}$$

where we have introduced the following new variables:

$$\tau=\omega t,\quad [v(I),s_I]=\Omega[V(I),S(I)] \tag{13a}$$

and

$$\omega=|a_2|/\sqrt{Ma_3},\quad \Omega=a_2/a_3\ ,$$
$$\alpha=a_1a_3/a_2^2,\quad \beta=c_2a_3/a_2^2\ , \tag{13b}$$
$$\delta=d_1a_3/a_2^2,\quad \eta=d_2a_3/a_2^2\ .$$

The new strain $S(I)$ is related to the displacement $V(I)$ through the relation

$$S(I)=V(I+1)-V(I)\ . \tag{14}$$

We assume that a_3 is positive and a_2 is nonzero. Moreover, the lattice spacing can be set to the unit without changing the results.

IV. EQUATIONS OF MOTION

The equations of motion for the transverse displacement $V(n)$ are easily obtained from the Lagrangian (12) and the definition of the discrete strain (14). However, it is more convenient to work with the equations governing the shear deformation $S(n)$. These equations read as

$$\ddot{S}(n)=\Delta^2[\sigma(n)-\Delta^+\chi(n)]\ , \tag{15a}$$

where we have set

$$\sigma(n)=\alpha S(n)-S^2(n)+S^3(n)$$
$$+\beta[S(n+1)+2S(n)+S(n-1)]\ , \tag{15b}$$

$$\chi(n)=\delta\Delta^-S(n)+\eta\Delta^-[S(n+2)+4S(n+1)+6S(n)$$
$$+4S(n-1)+S(n-2)]\ . \tag{15c}$$

Equation (15b) defines the discrete macroscopic stress, and the microscopic stress due to the bending forces is given by Eq. (15c). The operators Δ^- and Δ^+ hold for the backward and forward first-order finite differences defined by

$$\Delta^-f(n)=f(n)-f(n-1),\quad \Delta^+f(n)=f(n+1)-f(n)\ ,$$

respectively. Equation (15a) is a set of coupled nonlinear ordinary differential equations which governs the shear deformation traveling perpendicularly to the close-packed atomic planes. Note that the nearest four neighbors are involved in the shearing of the plane at n. In the discrete case, these equations are complicated to solve except for the linear problem which will be examined in Sec. VI. The strongly nonlinear feature of Eq. (15) can be tackled, however, by means of numerical simulations with appropriate initial and boundary conditions at the ends of the atomic chain. An alternative situation occurs in the case of the continuum approximation; this side of the problem will be studied in the following paper.

V. HOMOGENEOUS STATES OF DEFORMATION

We examine the lattice potential (12) for homogeneous strains $S(l)=S_0$. Then the potential per volume unit is reduced to

$$\mathcal{V}(S_0,T)=\tfrac{1}{2}A(T)S_0^2-\tfrac{1}{3}S_0^3+\tfrac{1}{4}S_0^4 , \tag{16}$$

where we have set

$$A(T)=\alpha+4\beta . \tag{17}$$

Note that the potential parts coming from the three-body interaction do not contribute to the potential (16) for the homogeneous states. In fact, it is not surprising that we obtain the free energy of the Landau type, where S_0 is merely the order parameter and the associated elastic modulus $A(T)$ defined in Eq. (17) corresponds to $(C_{11}-C_{12})/2$.[30] Furthermore, along with the Landau theory of phase transitions for ferroelastic crystals the elastic modulus A depends on temperature according to the Curie-Weiss law $A(T)=A_0(T-T_c)$, where T_c is some temperature of transition.[3] The free-energy expansion (16) possesses a cubic term which violates the usual Landau condition of symmetry,[31,32] but this extra term induces a first-order phase transition. If this term is absent, for some symmetry considerations, we must consider an expansion of the free energy (9) up to the sixth order in shear deformation.[33,34] We must note that the lattice potential for homogeneous deformations [Eq. (16)] deduced from the present lattice model is quite similar to that obtained by means of an irreducible representation of a functional of the symmetric strain tensor for the space group of the high-temperature phase [i.e., fcc $(m3m)$] and where the result has been reduced to the particular deformation characterized by the shear S.[18,21,35] The lattice energy is sketched in Fig. 2 for different values of A. For $A\geq\frac{1}{4}$, $S_0=0$ is the only stable minimum corresponding to the underformed lattice or the austenitic phase. Next, for $\frac{2}{9}<A<\frac{1}{4}$ the potential has a stable minimum at $S=0$ (austenitic state) and a metastable minimum at nonzero strain. When $0<A<\frac{2}{9}$ we still have two minima, but the minimum at $S=0$ is now metastable whereas the minimum at $S\neq 0$ is stable and it corresponds to the deformed lattice or the martensitic phase. Finally, if $A\leq 0$, only the nonzero strain minimum remains and the martensitic phase is predominant. The associated shear stress is given by

$$\sigma=\frac{\partial\mathcal{V}}{\partial S_0}=A(T)S_0-S_0^2+S_0^3 . \tag{18}$$

It is worth commenting on the *stress-strain relation* (18). The latter is not single-valued and this yields the notion of *hysteresis* which characterizes ferroelastic materials. For S small enough, in particular in the vicinity of the minimum $S=0$—austenitic phase—the material is *nearly linear* and the linear elasticity is valid. At lower temperature the material has a strongly nonlinear behavior and it is a so-called pseudoelastic displaying unstable region associated with the nonconvex parts of the elastic potential (16). At much lower temperature, the hysteresis is growing and a vanishing stress can be reached for a nonzero strain and the martensitic phase is then dominant. Macroscropic phenomenological models have been devoted to a complete study of this rich behavior[1,2,33] of which many technological applications are interesting. In the forthcoming sections, for convenience sake we prefer to use A as the transition parameter instead of temperature.

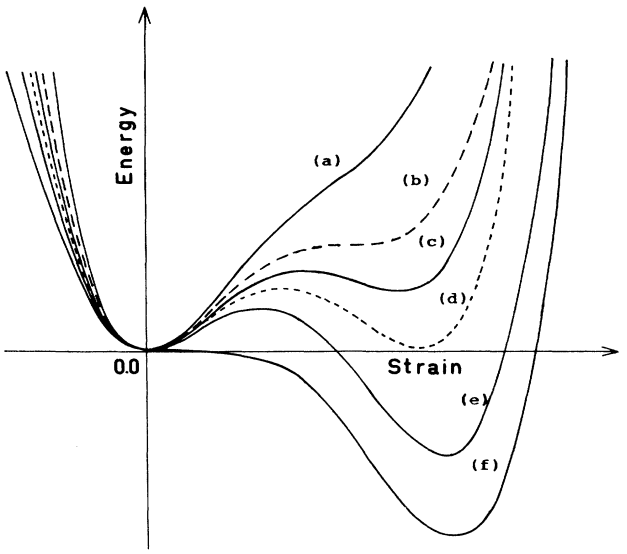

FIG. 2. Lattice energy for a homogeneous state of deformation. According to the value of A, curve (a) the high-temperature phase is stable ($A<\frac{1}{4}$), curve (c) there exists one austenitic stable phase and metastable martensitic phase ($\frac{2}{9}<A<\frac{1}{4}$), curve (e) metastable high-temperature phase and stable low-temperature phase ($A<\frac{2}{9}$), curve (f) ($A<0$) the martensitic phase is predominant. Particular cases for $A=\frac{1}{4}$ [curve (b)] and $A=\frac{2}{9}$ [curve (d)].

VI. ACOUSTIC-PHONON DISPERSION

Although we are interested in nonlinear excitations (see paper II), the linear problem is nonetheless instructive. We then consider the linearized equation (15) about a uniform deformation S_0. But we choose S_0 satisfying one of the minima of the lattice potential (16). S_0 is then given by

$$\begin{aligned} &S_0=0 \quad \text{if } A>\tfrac{1}{4} , \\ &S_0=0 \text{ or } S_0=\frac{1+\sqrt{1-4A}}{2} \quad \text{if } A\leq\tfrac{1}{4} . \end{aligned} \tag{19}$$

Small harmonic sinusoidal wave solutions traveling along the stacking direction can be looked for. This yields the dispersion relation for the linear waves

$$\begin{aligned} \left[\frac{\omega}{2}\right]^2=&[A(S_0)-4(\beta-\delta-16\eta)\sin^2(q/2) \\ &-128\eta\sin^4(q/2)+64\eta\sin^6(q/2)]\sin^2(q/2) , \end{aligned} \tag{20}$$

where

$$A(S_0)=A-2S_0+3S_0^2 \tag{21}$$

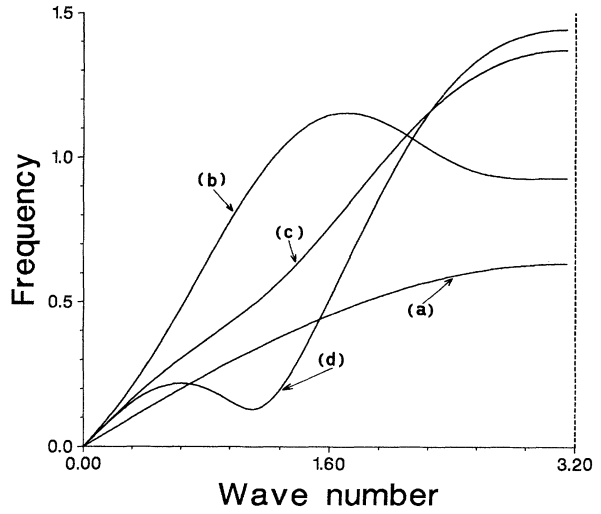

FIG. 3. Dispersion curves for the transverse-acoustic phonons in the [110] direction.

represents the induced elastic modulus in the martensitic phase. ω is the angular frequency and q is the wave number ($q \in [0,\pi]$). The dispersion relation curves are depicted in Fig. 3 for different values of the lattice parameters α, β, δ, and η, which places the importance of the competing interactions in evidence. The effects of these interactions can be examined more precisely if we consider the long-wavelength limit of the dispersion relation (20). For small q Eq. (20) can be expanded up to the fourth order

$$\omega^2 = A(S_0)q^2 - [A(S_0)/12 + (\beta - \delta - 16\eta)]q^4 + O(q^6) . \tag{22}$$

If we keep only the first term in (22), we recover the classical phonon dispersion of the transverse elastic waves where $\sqrt{A(S_0)}$ is the transverse elastic velocity when $A(S_0) > 0$. This is exactly the convexity condition of the lattice potential since $A(S_0) = (\partial\sigma/\partial S)_{S_0} = (\partial^2\Phi/\partial S^2)_{S_0}$ which is the effective shear elastic modulus induced in the martensitic phase. In addition, this condition is fulfilled since S_0 given by Eq. (19) is one of the minima of the lattice potential. The second term in (22) controls the convexity of the transverse-phonon branch. Curve (b) in Fig. 3 has an upward convexity at the long-wavelength region if the condition

$$A(S_0)/12 + (\beta - \delta - 16\eta) < 0 \tag{23}$$

is satisfied. This condition will be quite useful for the existence of coherent structures of the soliton type. Moreover, condition (23) depends firstly on the free energy of the Landau type (16) through $A(S_0)$ [see Eq. (21)] and secondly on the three-body interaction (through the parameters δ and η). Curve (a) differs slightly from the classical case. The dispersion branch (c) has a small bend at a nonzero wave number and this curve undergoes a softening at a nonzero wave number which can be interpreted as a precursor of martensitic transformation or premartensitic transitions.[22,24] The existence of a sharp dip in the transverse-acoustic-phonon dispersion curve [see Fig. 3(d)] at a high-symmetry point q_0 leads to the lattice instability against a perturbation with a wave vector in the vicinity of q_0, which is observed by the neutron-inelastic-scattering technique.[17,19,23] This produces a modulated lattice distortion within the parent phase with a period q_0 which is detected by electron microscopy and electron or x-ray diffraction.[24] Transmission electron micrographs exhibit a fine scale, diffuse, striated microstructures which are commonly referred to as "tweed" patterns developing within the parent phase (cubic phase).[7,23,24]

VII. CONCLUSIONS

The aim of the first part of this work was to build and study a lattice model including a fine-scale description for elastic domain patterns occurring in ferroelastic-martensitic transformations. Since our model is applied to proper ferroelasticity, the order parameter is properly defined by the strain tensor associated with the elastic transformation. In addition, comparison with the Landau theory of transition has been considered in order to identify the shear modulus $(C_{11} - C_{12})/2$. More precisely, we have presented a nonlinear model for cubic-tetragonal transformations. Although this work is mostly devoted to a one-dimensional model, we have pointed out the necessity of starting from a two-dimensional system leading to a one-dimensional version which contains the lattice anisotropy and competing interactions. The one-dimensional lattice system, which corresponds to a volume-preserving transformation, describes the shearing motion of the atomic planes $(1\bar{1}0)$ stacking in the [110] direction. It has been shown that the lattice potential [see Eqs. (9) or (16)] contains a third-order term with respect to the shear deformation which induces a first-order transition and we recover the well-known description of the ferroelastic crystals.[3,18,21,31] The Landau symmetry condition is not satisfied, but this is not surprising; indeed, even if scalar quantities are concerned in the model, the tensorial feature of the deformation is nonetheless present and nonlinear terms of the second order exist in the stress-strain relation.

The pertinent results of the microscopic model are (i) the partial softening of the transverse-acoustic phonon at nonzero wave number and (ii) the upward convexity of the dispersion branch in the vicinity of the long-wave length limit. These phonon behaviors given by the present model are observed by means of neutron-scattering techniques for various alloys such as Ni-Ti, In-Tl, Nb_3Sn, Fe-Pd just to quote few examples.[19,20,22,24] Although the discrete problem of nonlinear excitations is interesting and very important in the case of microtwinning effects, we will attack in paper II the quasicontinuum approximation in order to study movement of elastic domain structures as strain solitary waves.

ACKNOWLEDGMENTS

The Laboratoire de Modélisation en Mécanique is Unité Associée au Centre National de la Recherche Scientifique.

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