Stability of nonlinear structures in a lattice model for phase transformations in alloys

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The nonlinear dynamics of elastic twinning in martensitic-ferroelastic materials is presented on the basis of a two-dimensional lattice model. The model is suited to square-rectangle transformations characterized by two strain components. The microscopic model involves nonlinear and competing interactions emerging from interactions as a function of particle pairs and noncentral-type or bending forces. These interactions are of the most importance for the existence of nonlinear coherent structures made of elastic (martensitic) domains and twin boundaries. A special attention is devoted to the quasicontinuum approximation of the two-dimensional discrete system with the view of including the leading discreteness effects at the continuum description. This becomes particularly crucial for the stability of the lattice. Moreover, macrostresses and microstresses are placed in evidence where the contributions of the discreteness effects and bending forces or noncentral interactions are both considered. The emphasis is especially placed on the investigation of the complete two-dimensional system. Numerical simulations show that a moving martensitic band is unstable with respect to the transverse disturbances yielding thus localized structures consisting of disk-shaped domains. By means of a perturbative method a criterion of stability is found which involves the total energy of the system and parameters of the nonlinear structure. The conjecture of instability thus obtained is checked on the numerical simulations. The long-time evolution of the localized patterns is governed by an asymptotic equation of the Kadomtsev-Petviashvili type deduced from the quasicontinuum model. At length, an attempt at a comparison of the most pertinent results deduced from the proposed model with available experiments is made, which mainly confirms the physical basis of the model.

I. INTRODUCTION

Research in recent years has exhibited an increasing interest in complex spatial structures and nonlinear dynamics occurring in various fields of physics (periodic and localized patterns, spiral structures, vortices, etc.). The investigation of *nonlinear dynamics of spatiotemporal structures* has become a common necessity for numerous problems in physics such as focusing patterns in plasmas, modulated instability in convective fluid, magnetic flux in Josephson-junction transmission lines, or domain twinning in crystals.[1] The systems dispaying such behaviors are often met in hydrodynamics or reaction-diffusion equations and great progress has been achieved in the understanding of pattern formation and stability in these systems.[2] However, spatiotemporal pattern formations and their dynamics become useful in the description of the *evolution of defect distributions* and *propagation of ordered structures* in various problems of condensed-matter physics such as phase transitions.[3,4] Here, we are concerned with the dynamics and stability of nonlinear structures in two-dimensional systems taking place in *phase transformations in alloys* on the basis of *lattice models.* The main motivation of the present work is to understand how spatial structure formation and related dynamics arising at the *microscale* are able to organize the system at the *macroscale.* In other words, the global response of a material to stimuli at the specimen scale is the *cooperative* behavior of a complex dynamics taking place at a *mesoscale* halfway between the microscopic level and the experiment scale. For instance, structures made of elastic domains (transformed regions) and domain walls are usually observed experimentally by means of high-resolution electron microscopy,[5,6] and experimental works reveal a rich and complex crystalline morphology. These studies, although considered fundamental researches, appear now to be of technological importance for engineering physics.

We point out the interest of a *lattice model* because the latter possesses the most underlying physical ingredients that contribute to the formation of twinnings in alloys. In the present work we address particular attention to the nonlinear dynamics of elastic twin formation occurring in the *phase transformation of martensitic-ferroelastic type* in crystals.[7,8] The transformation is characterized by involving a lattice distortion, usually shear displacements. Moreover, the transformation is usually accompanied by twin formation and nucleation of different martensitic variants.[7,9,10] The dynamics of twin interfaces and twin bands, of which the stability seems to be very sensitive to the *discreteness effects* of the crystal, play a key role in the transformation. The nucleation process can be seen as a pretransformation phenomenon where modulated strain structures are developed within the high-temperature or parent phase, however, the *instability phenomena* can be considered as the *growth of martensitic phases,* thus producing localized structures. These microstructures are well described at an intermediate scale where the microscopic scale background provides competing interactions and strongly nonlinear lattice potentials. Static and dynamics studies of martensitic twinning have received particular attention because twinning formation and interface migration play a major role in *shape memory effect*. Different valuable and interesting models based on a continuum approach were proposed[11–14] in order to describe the structure of twin boundaries in ferroelastic and martensitic materials. Here, we also extend a lattice model[15] to a two-dimensional system and we examine in more detail a model previously studied in Refs. 15 and 16. Nevertheless, though the one-dimensional model has given pertinent results about the propagation of localized structures, describing the shearing motion of atomic planes, we can expect more striking results concerning the elastic structures for the two-dimensional system.

The first task of the work is the construction of the model itself; this is proposed in Sec. II. By considering a particular transformation involving only one displacement, we obtain the equations of motion for the microscopic system in Sec. III. Because this set of nonlinear difference-differential equations is not tractable as a discrete system, we derive, by using an interpolation method, the quasicontinuum model which incorporates the leading discreteness effects in Sec. IV. A short digression is made to the one-dimensional version in Sec. V, where we recall the most significant results provided by the model.[16] In Sec. VI, the two-dimensional model is examined and numerical simulations are performed on the microscopic model. Especially, localized and ordered structures, which emerge from an instability mechanism of an elastic solitary wave with respect to the transverse disturbances, are studied by using a perturbative technique, thus leading to a criterion of stability. A subsection is devoted to the derivation of an asymptotic model of the Kadomtsev-Petviashvili type. At length, some concluding remarks and further problems are evoked in Sec. VII.

II. LATTICE MODEL

A. The lattice deformations

Let us consider an atomic plane extracted from a cubic lattice (for instance, the fcc symmetry of In-Tl or Fe-Pd crystals undergoing a martensitic-ferroelastic transformation). The geometry of the lattice plane, in its underformed state, is made of squares parallel to the i and j directions (see Fig. 1). A particle of the plane is located by (i,j). After deformation of the lattice, the particles suffer displacements in the plane defined by $u(i,j)$ and $v(i,j)$, which are the displacements in the i and j directions, respectively. In previous works,[15–17] a model has been studied by using the system $(\mathbf{I},\mathbf{J})$ deduced from the system $(\mathbf{i},\mathbf{j})$ by a rotation 45° clockwise. A further step to the simplification consists in considering transformations of the lattice involving the displacement $u(i,j)$. Then, we define the following discrete deformations:

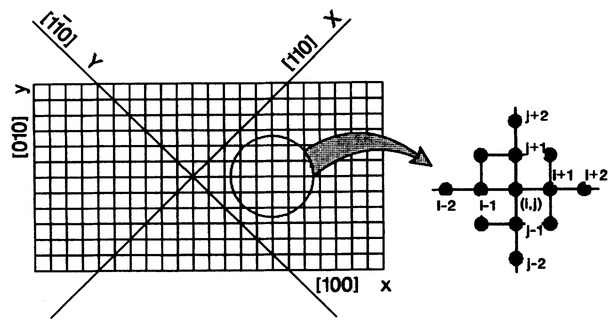

FIG. 1. Two-dimensional lattice model with the detail of interatomic interactions between the first and second neighbors in the i and j directions.

$$S(i,j)=u(i,j)-u(i-1,j)\ , \tag{1a}$$

$$G(i,j)=u(i,j)-u(i,j-1)\ . \tag{1b}$$

The first strain component (1a) denotes the elongational deformation and Eq. (1b) represents the pure shear.

B. Interatomic potentials

We assume that the particles interact via two types of interatomic potential. A first interatomic interaction between first-nearest neighbors is defined as a function of *particle pairs* in the i and j directions. The corresponding potential must describe homogeneous deformations with unstable, stable, or metastable regions according to the strength of the lattice forces. Next, we consider a second kind of interaction involving *noncentral forces* (or three-body interactions), which are equivalent to bond bending or torsional forces due to the long-range atomic interactions.[18,19] these interactions occur between *first- and second-nearest neighbors* and then allow us to introduce some competing interactions. Moreover, this amounts to describing, at the microscopic level, the resistance of the crystalline cell to twisting and bending. Along with somewhat general hypotheses about atomic interactions and the invariances of the lattice energy under translations and rotations,[20] the lattice energy must be a function of the relative particle displacements. Then, we can propose the following functional of the discrete deformations:

$$\mathcal{V}=\sum_{(i,j)}\{\Phi[S(i,j)]+\tfrac{1}{2}\beta[G(i,j)]^2+\tfrac{1}{2}\delta\left[[\Delta_L^+S(i,j)]^2+[\Delta_T^+G(i,j)]^2\right]$$
$$+\tfrac{1}{2}\eta[\{\Delta_L^+[S(i+1,j)+2S(i,j)+S(i-1,j)]\}^2+\{\Delta_T^+[G(i,j+1)+2G(i,j)+G(i,j-1)]\}^2]\}\ , \tag{2}$$

where we have set

$$\Phi(S)=\tfrac{1}{2}\alpha S^2-\tfrac{1}{3}S^3+\tfrac{1}{4}S^4\ . \tag{3}$$

The lattice energy (2) has been written in nondimensional units and the coefficients α, β, δ, and η are the parameters of the model. The first and second terms in Eq. (2) are the nonlinear and linear interactions emerging from the particle pair interactions. The lattice potential (3) corresponds to the expansion up to the fourth order of the interactions by particle pairs in the i direction (the elongation of the lattice). The linear part containing the lattice coefficient force β is deduced from the interactions by particle pairs in the I and J directions (the shearing of the lattice). The third and fourth parts of the lattice potential represent the noncentral interactions in the i and j directions between first- and second-nearest-neighboring particles, respectively. The operators Δ_L^+ and Δ_T^+ hold for the forward first-order finite differences in the i and j directions,

$$\Delta_L^+ f(i,j) = f(i+1,j) - f(i,j)$$

and

$$\Delta_T^+ f(i,j) = f(i,j+1) - f(i,j) \ .$$

Remarks. (i) It should be noticed that there exist some symmetries in the lattice model, indeed, if we swap u for $-v$ and we exchange the role played by i and j, we have the same lattice description. This means that the transformation characterized by the displacement $v(i,j)$ can be deduced from that described by $u(i,j)$ by a 90° rotation of the whole lattice. (ii) On the other hand, if we set $u=-V/\sqrt{2}$ and $v=V/\sqrt{2}$ where V is the lattice displacement in the J direction (omitting the indexes i and j), then we recover the particular transformation that we have studied in Refs. 15 and 17. Furthermore, it can be proved that the lattice energies associated with these different transformations take on the same form. (iii) A one-dimensional version of the model can be obtained by assuming transformation involving the displacement V along the J direction which depends only on I. This reduced one-dimensional model has provided interesting results concerning the shearing motion of the atomic planes along the stacking direction modeled by arrays of martensitic and austenitic solitary waves.[16,17] A short review of the main features of the one-dimensional version of the model will be presented in Sec. V.

III. EQUATIONS OF MOTION FOR THE DISCRETE SYSTEM

We add the kinetic energy

$$K = \sum_{(i,j)} \tfrac{1}{2}\dot{u}^2(i,j) \ , \tag{4}$$

to the lattice energy where the mass of the particles has been set to unity for ease of presentation. From the Hamiltonian ($H = K + V$) of the system we can write the equations of motion as

$$\ddot{u}(i,j) = \Delta_L^+ \Sigma_L(i,j) + \Delta_T^+ \Sigma_T(i,j) \ , \tag{5}$$

where we have defined

$$\Sigma_L(i,j) = \sigma(i,j) - \Delta_L^- \chi_L(i,j) \ , \tag{6a}$$

$$\Sigma_T(i,j) = \beta G(i,j) - \Delta_T^- \chi_T(i,j) \ , \tag{6b}$$

$$\sigma(i,j) = \alpha S(i,j) - S^2(i,j) + S^3(i,j) \ , \tag{6c}$$

$$\begin{aligned}\chi_L(i,j) = \Delta_L^+\{&\delta S(i,j) \\ &+\eta[S(i+2,j)+4S(i+1,j)+6S(i,j) \\ &+4S(i-1,j)+S(i-2,j)]\} \ ,\end{aligned} \tag{6d}$$

$$\begin{aligned}\chi_T(i,j) = \Delta_T^+\{&\delta G(i,j) \\ &+\eta[G(i,j+2)+4G(i,j+1)+6G(i,j) \\ &+4G(i,j-1)+G(i,j-2)]\} \ .\end{aligned} \tag{6e}$$

The operators Δ_L^- and Δ_T^- represent the backward first-order finite differences in the i and j directions. Equations (6a) and (6b) define the discrete macroscopic stresses due to the deformations $S(i,j)$ and $G(i,j)$ as a function of the discrete displacement $u(i,j)$ [see Eq. (1)]. The microscopic stresses emerging from the noncentral forces are given by Eqs. (6d) and (6e) and they are, in fact, functions of the discrete variations of the deformations in the i direction for $S(i,j)$ and in the j direction for $G(i,j)$. Note that the stress (6c) derives from the potential (3) and it is a nonlinear relation of the strain $S(i,j)$. The investigation of the set of the coupled nonlinear ordinary differential equations which governs the displacement $u(i,j)$ is not manageable, therefore we must consider the continuum approximation.

IV. QUASICONTINUUM MODEL

In order to describe, at the continuum scale, the lattice dynamics, we consider an interpolation method that incorporates the *leading discreteness effects* due to the lattice. The procedure is based on the Fourier image of the discrete quantities restricted to the first Brillouin zone in order to smooth out the Fourier components with increasing oscillations.[16,18,21,22] To this end, we materialize the procedure by taking the Fourier image of Eq. (5), which has been written for the deformation S. Then we arrive at

$$\omega^2\hat{S}(p,q,\omega) = 4\sin^2(p/2)\hat{\Sigma}_L + 4\sin^2(q/2)\hat{\Sigma}_T \ , \tag{7}$$

where we have set

$$\hat{\Sigma}_L = \hat{\sigma} + 4\delta\sin^2(p/2)\hat{S} + 64\eta\sin^2(p/2)\cos^2(p/2)\hat{S} \ , \tag{8a}$$

$$\hat{\Sigma}_L = \beta\hat{S} + 4\delta\sin^2(q/2)\hat{S} + 64\eta\sin^2(q/2)\cos^2(q/2)\hat{S} \ , \tag{8b}$$

where $\hat{S}(p,q,\omega)$ is the Fourier image in space and time of the deformation $S(i,j)$ and $\hat{\sigma}$ is that of the stress (6c). Equations (8a) and (8b) also define the Fourier images of the stresses given by Eqs. (6a) and (6b) by accounting for Eqs. (6d) and (6e). At this stage of the work, we assume that the displacement and deformation are slowly varying over the lattice spacing. Accordingly, we can consider the *long-wavelength limit* of Eqs. (7) and (8). Then, by expanding Eq. (8) and Eqs. (8a) and (8b) with respect to p and q up to the fourth order, we can rewrite Eq. (7) as

$$\omega^2(1+p^2/12+q^2/12)\hat{S} = p^2\hat{\Sigma}_L + q^2\hat{\Sigma}_T \ , \tag{9a}$$

where the new stresses are then given by

$$\hat{\Sigma}_L = \hat{\sigma} + p^2\bar{\delta}\hat{S} + \tfrac{1}{12}\alpha q^2 \hat{S} \ , \tag{9b}$$

$$\hat{\Sigma}_T = \beta\hat{S} + q^2\bar{\delta}\hat{S} + \tfrac{1}{12}\beta p^2 \hat{S} \ . \tag{9c}$$

We have set $\bar{\delta} = \delta + 16\eta$. Some comments about Eqs. (9b) and (9c) are in order. Since the expansion has been done up to fourth order we must include, for consistency, the fourth-order terms emerging from the linear parts of the macroscopic stresses σ and βS, that is, $(\alpha+\beta)p^2q^2\hat{S}/12$. The latter is split into two parts appearing in Eqs. (9b) and (9c). Now, by taking the inverse Fourier image of Eqs. (9a)–(9c), we readily obtain the equation of motion for the continuous deformation $S(x,y,t)$, which is

$$Q_{tt} = \Sigma_{Lxx} + \Sigma_{Tyy} \ , \tag{10a}$$

with

$$Q = S - \Delta S/12 \ , \tag{10b}$$

$$\Sigma_L = \sigma(S) - \bar{\delta} S_{xx} - \tfrac{1}{12}\alpha S_{yy} \ , \tag{10c}$$

$$\Sigma_T = \beta S - \bar{\delta} S_{yy} - \tfrac{1}{12}\beta S_{xx} \ . \tag{10d}$$

The stresses are then defined by Eqs. (10c) and (10d) where the first parts are the macrostresses and the second and third terms stand for the microscopic stresses due, first, to the noncentral interactions (terms in $\bar{\delta}$) and, second, to the discreteness effects (terms in α and β). On the other hand, we notice the particular form of the inertial term in Eq. (10b), which comes from the fine description of the lattice dynamics[16] (Δ is the Laplacian operator in the lattice plane).

The equation of motion (10), when it is written with respect to the displacement u, can be derived from the following Hamiltonian

$$H = \int_{\mathcal{D}} (K + \Phi) dx\, dy \ , \tag{11}$$

where we have defined the density of kinetic energy

$$K = \tfrac{1}{2}\left[u_t^2 + \tfrac{1}{12} S_t^2 + \tfrac{1}{12} G_t^2 \right] , \tag{12}$$

and the potential Φ is given by

$$\Phi = \tfrac{1}{2}\alpha S^2 - \tfrac{1}{3}S^3 + \tfrac{1}{4}S^4 + \tfrac{1}{2}\beta G^2 + \tfrac{1}{2}\bar{\delta}[(S_x)^2 + (G_y)^2] + \tfrac{1}{24}(\alpha+\beta)[(S_y)^2 + (G_x)^2] \ . \tag{13}$$

In addition, the deformations are

$$S = u_x, \quad G = u_y \ . \tag{14}$$

We remark that the elastic potential (13) is similar to the Ginzburg-Landau free energy for ferroelastic materials involving two strain components.[23] However, the deformation S can be considered, here, as the primary order parameter associated with the first-order phase transition and the elastic coefficient α depends on the temperature according to the Curie-Weiss law.[24,25] The behavior of the material is therefore linear with respect to the second strain component G. Other elastic potentials of the Ginzburg-Landau type, including strain gradients, have been considered depending on the crystal symmetry in order to describe twinning in martensitic materials.[11–13,26]

V. REDUCTION TO THE ONE-DIMENSIONAL MODEL

(a) Here we want to stress the most significant results for the lattice model and its quasicontinuum counterpart when the displacement u depends only on the x coordinate. We record below the main equations and solutions of the one-dimensional model, but the reader can refer to papers discussing the one-dimensional system.[15,16] The equations of motion for the deformation $S(i) = u(i) - u(i-1)$ take on the form

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

where $\sigma(i)$ is the discrete macrostress defined by Eq. (6c) and $\chi(i)$ is still provided by Eq. (6d), but the second index j does not exist. The operator $\Delta = \Delta^-\Delta^+$ is the second-order finite difference in the i direction. We recover the different features of the original two-dimensional lattice emerging from the bending forces or noncentral interactions.

(b) Now, we can reach the quasicontinuum model by reducing directly Eqs. (10a)–(10c) to the x direction. By integrating with respect to x, we arrive at the equation for the displacement u,

$$P_{tt} = \Sigma_x \ , \tag{16a}$$

where we have set

$$P = u - S_x/12 \ , \tag{16b}$$

$$\Sigma = \sigma(S) - \chi_x \ , \tag{16c}$$

$$S = u_x \ . \tag{16d}$$

The macrostress and microstress derive from the elastic potential (13) for which $G = 0$ and the deformation S is now a function of x. Then, we can write

$$\sigma = \partial\Phi/\partial S, \quad \chi = \partial\Phi/\partial S_x \ . \tag{17}$$

(c) The one-dimensional version enables us to discuss a wide range of solutions to Eqs. (16a)–(16d).[16,17] Then, we have interesting situations; among them we can quote the following: (i) Modulated (almost sinusoidal) strain structures. (ii) Array of solitons describing a spatially arranged structures made of periodic martensitic plates. Moreover, the periodic modulated strain structure can be considered as an incommensurate phase embedded in the parent phase.[26,27] (iii) Array of kink-antikink pairs interpreted as periodic arrangement of large martensitic bands endowed in the austenitic phase. (iv) An austenitic solitary wave moving in a martensitic matrix which corresponds to a martensitic phase partially transformed. (v) A static domain wall between an austenitic and martensitic domains. (vi) A strain solitary wave corresponding to a small layer of martensite moving in the undeformed lattice. The latter case is examined in more detail below.

We now focus on the particular case (vi) which will interest us in the forthcoming sections. When looking for traveling solutions we can obtain an exact solution to Eqs. (16a)–(16b) and the associated strain reads as[16]

$$S(\xi)=\frac{S_m}{1+P\sinh^2(Q\xi)} , \tag{18a}$$

where we set

$$\xi=x-x_0-ct , \tag{18b}$$

$$c^2=\alpha-S_mS_0/2 , \tag{18c}$$

$$P=1-S_m/S_0 , \tag{18d}$$

$$Q^2=S_mS_0/8\gamma , \tag{18e}$$

$$\gamma=\bar{\delta}-c^2/12 . \tag{18f}$$

We have introduced $S_0=\frac{4}{3}-S_m$. We notice that the solitary wave velocity is strongly dependent on the wave amplitude S_m. Furthermore, the characteristic width of the excitation is mostly controlled by γ, which contains itself the velocity c [see Eq. (18f)]. However, the existence of the solution (18) is guaranteed if constraints on the amplitude S_m are met. The conditions of existence must guarantee that the velocity is real and such that $|c|<\sqrt{\alpha}$ for $\alpha>0$ and that P is positive as well as γ. It is worthwhile noting that these conditions are equivalent to that of the *upward convexity,* at the long-wavelength region, of the *dispersion branch for the linear mode* derived from the discrete system [see Eq. (11)].[15] This upward convexity of the dispersion phonon branch has been identified for the In-Tl material,[28] and this turns out to be crucial for the nonlinear analysis, though this condition has been obtained from the linear problem. This condition is merely given by $\bar{\delta}-\alpha/12>0$. In addition, the amplitude S_m must be smaller than $\frac{2}{3}$. The profile of the solution (18a) computed from the macroscopic model is sketched in Fig. 2 and it corresponds to a localized martenistic layer or strain solitary wave in an austenitic matrix. This can be interpreted as the formation of small platelike regions of the tetragonal phase in the austenitic (cubic) phase. Such structures are commonly observed by means of electron microscopy in various alloys such as Ni-Ti, Fe-Pd, In-Tl, etc.[9,29]

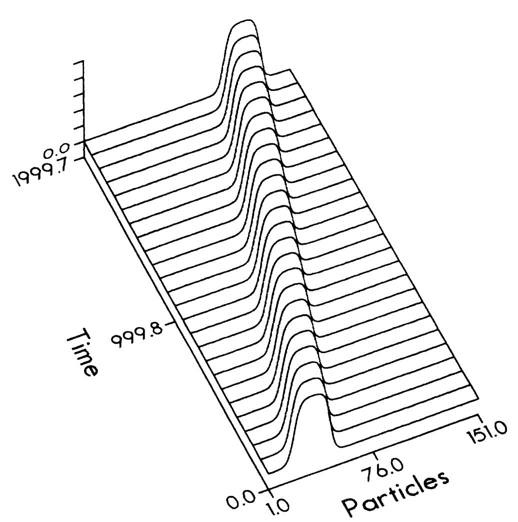

FIG. 2. One-dimensional lattice model: dynamics of a strain (martensitic) solitary wave moving on the undeformed phase.

VI. TWO-DIMENSIONAL ANALYSIS

A. Numerical simulations

Let us start first with the numerical investigations of the two-dimensional problem. We are searching for the instabilities caused by the dimensionality of the system, that is, *the instabilities with respect to the transverse disturbances* which do not exist, of course, for the one-dimensional version. On the other hand, a question can arise, what are the new spatial structures emerging from the instability process, and the problem is to know whether or not they are coherent and stable. More practically, we consider a band-shaped elastic domain traveling on the untransformed lattice as described by the solution to the one-dimensional problem [see Eq. (18)], and homogeneous in the other direction. This solution is used as the initial condition and it is nevertheless the solution to the two-dimensional problem. The numerical scheme is provided simply by the set of difference-differential equations (5) and (6). In addition, we consider pseudoperiodic boundary conditions on the left and right sides of the lattice and periodic conditions on the lower and upper boundaries. The numerical simulations are performed by using some estimates computed from the coefficients of the In-Tl alloy. The nonlinear part (3) of the lattice potential (2) can be rewritten in physical units by setting

$$\varphi(e)=\tfrac{1}{2}A_1e^2+\tfrac{1}{3}Be^3+\tfrac{1}{4}Ce^4 . \tag{19}$$

The dimensionless units are obtained with $\varphi=(B^4/C)\Phi$, $e=(|B|/C)S$, and $\alpha=A_1C/B^2$. The coefficients of the energy are such that they can be connected with those of a Landau free-energy expansion for crystals of $m3m$ cubic class.[23] Then, we have

$$A_1=(C_{11}-C_{12})/2 ,$$

$$B=(C_{111}-2C_{112}+2C_{123})/8\sqrt{3} ,$$

and

$$C=(C_{1111}-4C_{1112}+3C_{1122})/23 .$$

Moreover, the coefficient β in (2) can be calculated from the shear elastic modulus C_{44} and we have $\beta=C_{44}(C/B^2)$. For the In-21 at. % Tl alloy we obtain $A_1=0.12\times10^{11}$ dyn/cm^2 at $T=315.1$ K, that is, just above the transition ($T_0=314$ K), $B=-5.12\times10^{10}$ dyn/cm^2, $C=1.94\times10^{12}$ dyn/cm^2, and $C_{44}=0.75\times10^{11}$ dyn/cm^2.[24,30,31] These numerical coefficients allow us to compute those of the dimensionless free energy and we have $\alpha=0.02$, and $\beta=0.18$. In addition, the corresponding spontaneous shear at the phase transition is $e_0=0.026$. Insofar as the coefficient $\bar{\delta}=\delta+16\eta$ of the gradient terms is concerned, we take $\bar{\delta}$ such that the band thickness is $\Delta\simeq11-12$ lattice spacings,[29] this leads to $\bar{\delta}=0.25$. Then, we choose $\delta=0.252$ and $\eta=-0.002$. At the microscopic scale we should consider the thermal noise. But, here, the thermal fluctuations have not been accounted for since the system is not supposed to be coupled to a heat bath. In addition, the amplitude of the strain band is $S_m = 0.12$, which, in turn, yields the velocity $c = 0.327$.

The results of the numerical investigations are collected together in Fig. 3. Figure 3(a) represents the grey-shaded contour map for the deformation $S(i,j)$ at the initial time. This is a localized deformation in the x direction and homogeneous in the y direction. Some time later, some perturbations occur along the transverse direction while the deformation is moving in the x direction as depicted in Fig. 3(b). In fact, at the beginning of the instability process, the amplitude of the strain is modulated in time and space. The instabilities are growing and this means that the nonlinear elastic structure is no longer stable with respect to the transverse disturbances. After a lapse of time, a *localized elastic structure* is then produced. The resulting pattern is shown in Fig. 3(c) and we can see very clearly a *disk-shaped structure.* The latter is very robust and stable for a long time. This coherent structure moves in the x direction with almost the same form and a constant velocity, as shown in Fig. 3(d). From the numerical investigation we can extract some characteristic estimates for the localized structure shown in Figs. 3(c) and 3(d). In particular, the velocity of the moving structure is almost uniform ($V = 0.3$) and it is a little bit less than the velocity of the initial deformation ($c = 0.327$). In addition, the characteristic extent of the pattern is 6.5 and 15.7 lattice spacings in the x and y directions, respectively. Similar results have been obtained by considering a transformation characterized by the displacement V along a diagonal direction.[17]

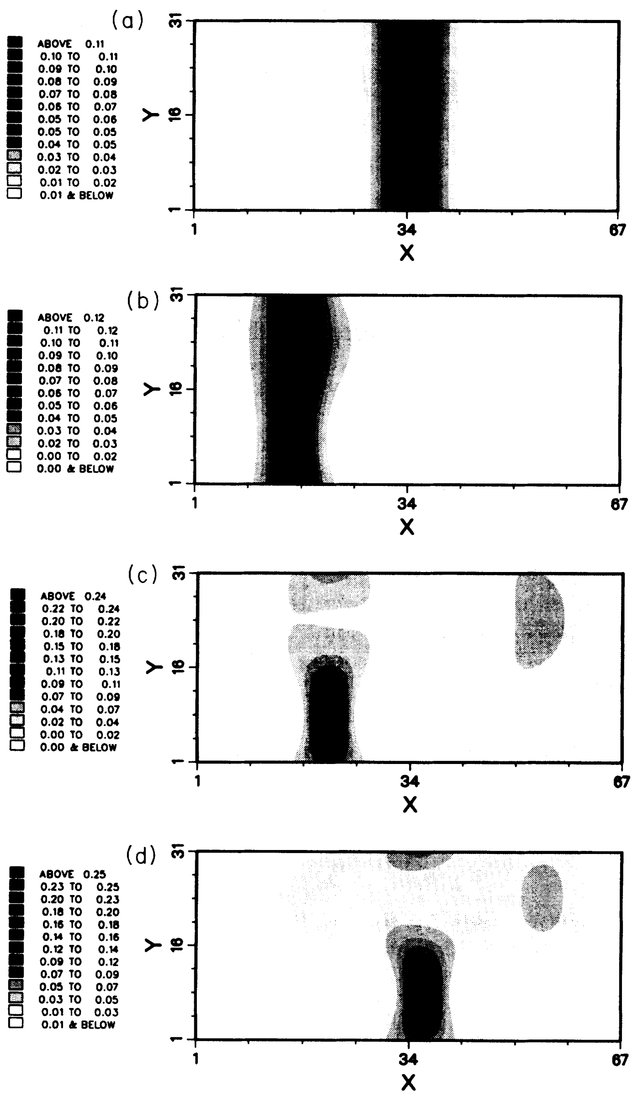

FIG. 3. Instability mechanism of a strain band structure moving on a two-dimensional lattice and formation of a localized coherent structure: (a) initial condition, strain band moving in the x direction and homogeneous in the y direction, (b) transverse modulations are developing along the transverse direction, (c) formation of a localized structure emerging from the instability, and (d) evolution of the coherent localized structure a long time later.

B. Stability of the nonlinear structure

The numerical simulations presented in the previous section inform us about the possible instabilities and their evolution as time increases. However, in order to understand the instability mechanism, we must know the parameters that play an important role in the instability process. The physical meaning of the instability is that the strain solitary wave velocity decreases with increasing amplitude according to Eq. (18c). Then, for a strain band weakly modulated along the transverse direction, the low-amplitude sections go faster than the high-amplitude sections [see Fig. 3(b)], and this effect results in a sort of self-focusing phenomenon. Accordingly, the evolution of small amplitude perturbations is growing and the formation of steady localized structures emerges. Specifically, a straightforward algebra based on *multiple scale technique,* which consists of finding an equation for the deformation amplitude perturbation, leads to an instability criterion. A similar technique has been used for another problem.[17] Then the nonlinear solution (18) is, indeed, *unstable* against the bending of the strain band whenever

$$\partial H / \partial S_m > 0 \ . \tag{20}$$

From the physical point of view, the instability occurs when the total energy of the system is increased as the strain amplitude. The regions of stability are shown in Fig. 4 (shaded areas) in the plane of the total energy versus strain amplitude when the parameter α is varied. Similar problems about instabilities and perturbation techniques have been met in a wide range of physical problems (plasma physics, crystal growth, gravitational waves in fluids, dynamics of fronts, etc.). Such instability effects and multiple scale methods have been considered in the context of two-dimensional weakly nonlinear waves modeled by the Kadomtsev-Petviashvili equation, nonlinear acoustic wave equation, or Schrödinger equation, for instance.[32,33] Returning to the numerical simulations, the computed total energy associated with the strain band is $E_{tot} \simeq 0.277$ (this quantity is conserved during the simulation). The corresponding energy density per surface is then $H \simeq 10^{-3}$. We can check easily that the points $S_m = 0.12$ and $H \simeq 10^{-3}$ do lie in the instability

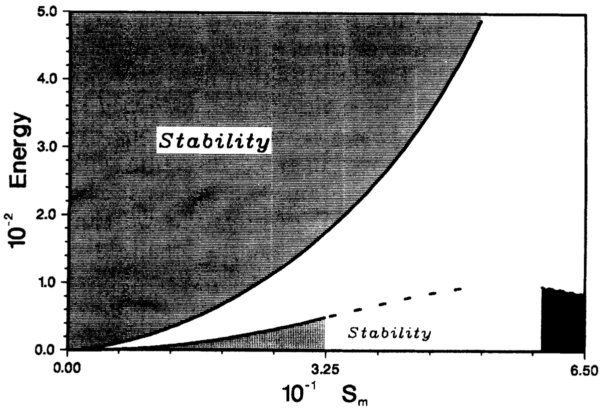

FIG. 4. Regions of stability (or instability) of a strain solitary wave with respect to the transverse direction in the two-dimensional system. The instability criterion is given by Eq. (20).

region of Fig. 4. Moreover, we have checked numerically that, if we choose a point in the stable regions, the instability growth does not occur at all.

C. Asymptotic model

In order to understand more precisely the *evolution of the localized structures over a large scale of time* and for *a weakly nonlinear* medium, we must consider here an asymptotic equation derived from the quasicontinuum model (10). Starting with the equation of motion (7) in the Fourier space we expand it for long wavelength up to fourth order. Then, we arrive at

$$(\omega^2-\alpha p^2)\hat{S}=\beta q^2\hat{S}+p^2\hat{\sigma}_{\rm NL}+p^4(\bar{\delta}-\alpha/12)\hat{S}+q^4(\bar{\delta}-\beta/12)\hat{S}\ , \tag{21}$$

where we have made use of Eqs. (8a) and (8b) for the definitions of the stresses. Moreover, the Fourier image of the macrostress $\hat{\sigma}$ has been broken into the linear part $\alpha\hat{S}$ and nonlinear part $\hat{\sigma}_{\rm NL}$. The latter corresponds to the Fourier image of $\sigma_{\rm NL}=-S^2+S^3$. Now, we suppose a *weak nonlinearities* and *slow time* variable and *stretching space* variables by setting

$$\hat{\sigma}_{\rm NL}=\epsilon\hat{\Sigma}_{\rm NL}\ , \tag{22a}$$

$$p=\epsilon^{1/2}P\ , \tag{22b}$$

$$q=\epsilon Q\ , \tag{22c}$$

$$\omega+vp=\epsilon^{3/2}\Omega\ , \tag{22d}$$

where the velocity $v=\sqrt{\alpha}$ ($\alpha>0$ is supposed to be true) denotes the acoustic wave velocity in the x direction. Here, ϵ is a small parameter associated with the nonlinear terms. At the lower order in the small parameter ϵ, namely, the second order, the Fourier image of the equation of motion (21) takes on the new form

$$-2v\Omega P\hat{S}=Q^2\beta\hat{S}+P^2\hat{\Sigma}_{\rm NL}+P^4D\hat{S}\ , \tag{23}$$

where we have set $D=\bar{\delta}-\alpha/12$. By introducing new real variables $T=\epsilon^{3/2}t$, $\xi=\epsilon^{1/2}(x-vt)$, and $Y=\epsilon y$ corresponding to the Fourier variables Ω, P, and Q, respectively, we can go back to the real-space representation by taking the inverse Fourier transform. The equation of motion thus obtained can be readily written as

$$[\Psi_T+(\Psi^2-\Psi^3)_\xi+D\Psi_{\xi\xi\xi}]_\xi=\beta\Psi_{YY}\ , \tag{24}$$

where the change of variable T into $-T/2v$ has been considered in order that Eq. (24) casts into a standard form. In addition, since the inverse Fourier image of $\hat{S}(P,Q,\Omega)$ is $\Psi(\xi,Y,T)$ that of $\hat{\Sigma}_{\rm NL}$ is then $-\Psi^2+\Psi^3$. The coefficient D of the dispersive term includes the discreteness effects of the lattice. Moreover, this coefficient can be negative if $\alpha>\bar{\delta}12$. Then, the long-time evolution of the nonlinear structure is governed by Eq. (24), which is of the *Kadomtsev-Petviashvili type* (KP equation). Nevertheless, the standard KP equation contains only the first nonlinear term.[33-35] In the framework of plasma physics the classical KP equation suffers transverse instabilities according to the sign of the dispersive terms and it possesses, moreover, soliton solutions.[35]

Equation (24) has a Hamiltonian structure

$$\Psi_T=\frac{\partial}{\partial\xi}\frac{\delta H}{\delta\Psi}\ , \tag{25}$$

with the Hamiltonian

$$H=\int[\tfrac{1}{2}D(\Psi_\xi)^2+\tfrac{1}{2}\beta(\varphi_Y)^2-\Psi^2+\Psi^3]d\xi\,dY\ , \tag{26}$$

where $\varphi_\xi=\Psi$. Localized solutions to Eqs. (24) or (25) can be searched for in the form $\Psi=\Psi(\xi-ct,Y)$ which decreases in all directions, the solution moving with the velocity c in the ξ coordinate. In addition, the quantity (the momentum)[36]

$$J=\int\Psi^2d\xi\,dY \tag{27}$$

is conserved. It can be seen that a localized solution to Eq. (24) is a stationary point of the Hamiltonian H for fixed J. The stability problem of the localized solution can be investigated by using Lyapunov theorem and, accordingly, the *boundedness of the Hamiltonian* from below guarantees the *stability* in the same way as for the classical KP equation.[34,35] On the other hand, a qualitative argument for stability can be found by introducing the characteristic length L of the localized structure. The characteristic length must be such that J remains, of course, invariant. In such a case the dispersion prevails on the nonlinearity and therefore singularities (divergence of some integrals) are forbidden. This explains the fact that the localized structure as shown in Figs. 3(c) and 3(d) is particularly stable and persists for a long time.

VII. CONCLUSIONS

In the present study we have proposed a lattice model and its quasicontinuum approximation with the view of understanding and describing the formation of nonlinear structures of elastic domain type involved in phase transformation (i.e., martensitic/ferroelastic transformations). The model is restricted to a cubic-tetragonal transformation and can be applied to alloys such as In-Tl, Fe-Pd, Ni-Al, and other ones which usually exhibit a first-order phase transition characterized by a lattice deformation (displacive transformations). Moreover, a particular emphasis is placed on the continuum approximation yielding the quasicontinuum model. The latter includes the most important discreteness effects and describes at best the lattice dynamics at the continuum level. On the other hand, the importance of the competing interactions (interactions by pairs and noncentral forces) for the twinning dynamics has been pointed out and particularly favors interesting coherent localized solutions. The collective contribution of both noncentral interactions and discreteness effects is in fact twofold; it triggers first the instability process of an elastic domain band with respect to its bending and it favors the stability of the localized structure thus produced.

The most relevant parts of the work lie in the elaboration of a two-dimensional lattice model allowing a rather fine description of nonlinear structures. The study provides some important results concerning the domain formation, that is, a structure made of disk-shaped or oval elastic domains of very rich morphology. The localized structure is the result of an instability process of the one-dimensional solution which describes a martensitic band. Moreover, a simple criterion for instability is found and can be obtained by means of the total energy of the system. Numerical investigations are carried out with the help of the equations of the microscopic model and allow us to check the physical conjectures. Here, the structure formation can be interpreted as the microtwinning of martensitic domains in the austenitic phase or as a nucleation mechanism of ferroelastic domains in alloys.[37,38] Localized elastic structures are commonly observed in high-resolution electron micrographs for a large variety of materials (e.g., Fe-Pd, In-Tl, Fe-Ni-C, etc.).[9,29] These structures are quite similar to those of the formation of bubblelike domains, lenticular or ellipse-shaped twins in ferroelectric materials.[39] An interesting point of the model is that we have derived an asymptotic model for the long-time evolution of the nonlinear structure. This model is then governed by an equation of the Kadomtsev-Petviashvili type and the problem of the stability of the localized solution is then solved.

It should be noticed that in contrast with models based on interface dislocations discussed by metallurgists, a number of valuable and interesting models using the soliton concept have been proposed.[11–13] These models, starting with the full nonlinear elasticity theory including strain gradient, attempt to describe moving coherent twin boundaries in martensitic materials. These works have placed kink-type solitary twin boundary and solitary domain wall in evidence for a continuum model. Although our approach seems to be different, some results dealing with domain structure are similar, in particular for the reduced one-dimensional models.[16,17] However, in the present study, we have pointed out the effects of the dimensionality of the problem and real two-dimensional localized strain patterns are found.

Further extensions of the model are worthwhile examining. For instance, *modulated structures* or quasisinusoidal strain waves made of periodic arrangements of elastic domains are of great physical interest. This problem can be related to commensurate-incommensurate transitions. We can introduce the displacement along the j direction, in this case the transformation is then characterized by two displacement components so that we can expect more complex patterns exhibiting the nucleation and growth of the topological defects. The *very discrete nature of the microscopic model* is a particularly difficult task if the continuum approximation is not considered. Nevertheless, a complete study of the microscopic feature of the model could be undertaken by introducing appropriate modifications in the lattice potential description, and this should confirm the richness of the lattice model. An extension of the model to a full three-dimensional system can be envisaged as well. Some of these problems will be presented in future work.

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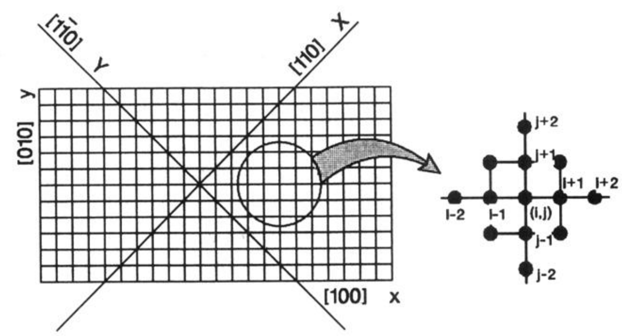

FIG. 1. Two-dimensional lattice model with the detail of interatomic interactions between the first and second neighbors in the *i* and *j* directions.

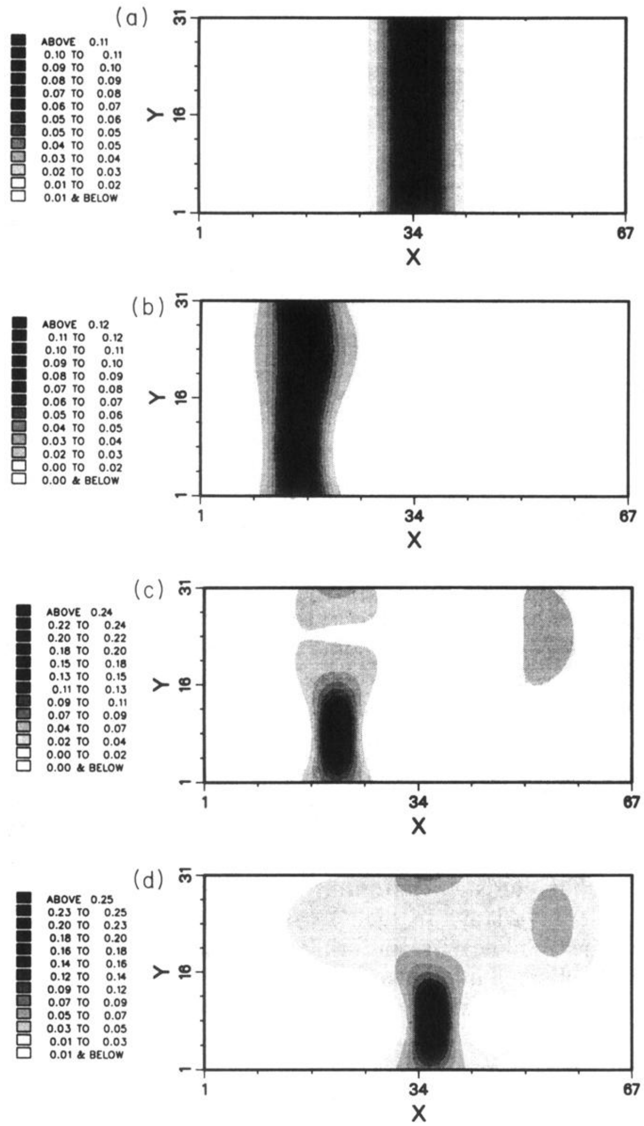

FIG. 3. Instability mechanism of a strain band structure moving on a two-dimensional lattice and formation of a localized coherent structure: (a) initial condition, strain band moving in the x direction and homogeneous in the y direction, (b) transverse modulations are developing along the transverse direction, (c) formation of a localized structure emerging from the instability, and (d) evolution of the coherent localized structure a long time later.

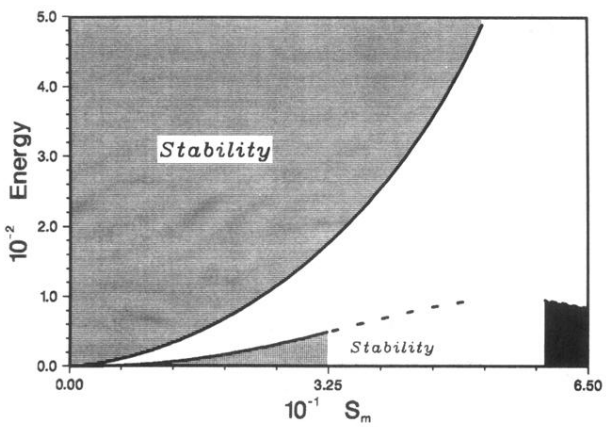

FIG. 4. Regions of stability (or instability) of a strain solitary wave with respect to the transverse direction in the two-dimensional system. The instability criterion is given by Eq. (20).