Stability of solitary-wave pulses in shape-memory alloys

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Within the framework of a one-dimensional continuous Ginzburg-Landau theory, pulselike solitary waves in shape-memory alloys are investigated. By neglecting heat conduction, internal friction, and external volume forces, but including shear-strain and strain-gradient contributions in addition to the Landau internal energy, a simple equation of motion is derived for the displacement of the atomic planes. It is shown that it has pulselike solitary-wave solutions for both the austenitic and the martensitic phase. The stability of the solitary pulses is investigated by the Liapunov method. Stability functionals are presented and analyzed. In the parameter regions where they do not satisfy the Liapunov criteria for stability, instability can be proved by variational methods. Thus, necessary and sufficient stability criteria are available for the existing pulselike solitary waves in shape-memory alloys. The criteria and their physical consequences are discussed.

I. INTRODUCTION

The shape-memory effect and related phenomena such as pseudoelasticity and ferroelasticity are due to a firstorder martensitic phase transition.¹ The latter is a special type of displacive phase transitions with a significant shear strain of the unit cell and a rather small change of the volume, whereas the rearrangement of the atoms within each cell ("shuffle") is secondary. A more detailed description of the physical phenomena can be found, e.g., in Ref. 2 and the references therein. At high temperatures most of the crystals have a cubic lattice. Typical are ordered bcc structures such as B2 (e.g., CuAl, NiTi, and AuCd) or $D0_3$ (e.g., CuAlNi and CuAlZn), but the fcc lattice occurs also (e.g., InTl). This high-temperature phase is called austenite. The low-temperature phase (martensite) typically shows orthorhombic (e.g., for CuAl, CuAlZn, CuAlNi, AuCd, CuAuZn₂, NiTi, etc.) or tetragonal (e.g., for InTl) symmetry. In order that the habit plane, i.e., the contact plane between martensite and austenite, is stress free on a macroscopic scale, martensite occurs in a twinned microstructure. Since in shapememory alloys twinning takes place on the scale of the lattice, a rather complex stacking sequence of closepacked planes is observed. Due to the extremely fine twinning, the habit-plane motion is reversible, thus enabling the shape-memory effect.

For the cubic-to-tetragonal martensitic phase transition Barsch and Krumhansl³ established a three-dimensional Ginzburg-Landau theory which shows kink-type solitarywave solutions representing moving plane twin boundaries. In their theory, elastic energy depends on appropriate strain tensor components up to fourth order and, in addition, on strain-gradient terms up to second order. For a square-rectangular martensitic transformation a Ginzburg-Landau theory was investigated by Jacobs.⁴

His two-dimensional (2D) theory models both cubic-totetragonal as well as cubic-to-orthorhombic transformations. In order to describe a first-order transition in a one- or two-dimensional theory, elastic energy has to comprise strain terms of second, fourth, and sixth order as well as strain-gradient terms of second order. The plane domain wall solutions in the 2D theory are essentially one-dimensional,⁴ i.e., they are identical to domain wall solutions resulting from a one-dimensional Ginzburg-Landau theory.⁵ So the one-dimensional theory yields the most important solutions of the 2D version already. Furthermore, it allows for pulselike solitary-wave solutions.⁶ A discrete version of a one-dimensional (1D)theory was investigated by Suzuki and Wuttig.⁷ Using for the energy an even polynomial of the sixth degree they numerically integrated the equation of motion for a lattice with periodic boundary conditions to find moving martensitic nuclei in an austenitic matrix.

The purpose of the present paper is to investigate, in the framework of a 1D continuous Ginzburg-Landau theory, the pulselike solitary waves in shape-memory alloys. Such an investigation requires a thorough discussion of the relevant physical models and their solutions. Very important for the development of a possible soliton scenario is the answer to the question of the stability of the calculated solitary waves. This topic will be a central point of this investigation.

The problem of stability of a nonlinear solution can be attacked in various ways with different pretensions. The mostly used method is the discussion of the corresponding linearized eigenvalue problem. It is generally simple but it has the disadvantages of using (often wrong) completeness arguments and, in addition, of ignoring the problem of nonlinear (in)stability. The more appropriate method seems to us the Liapunov method.⁸ When stability functionals can be found (satisfying the Liapunov criteria including the so-called convexity conditions), sufficient criteria for nonlinear stability will be available. However, as long as no additional arguments are presented, there is no proof that the criteria are also necessary. This task requires in general a tedious (compared to the less accurate linearized eigenvalue analysis) variational analysis. In the past⁹ it could be shown however that for solitonlike systems, a combination of the Liapunov method and variational procedures very often leads indeed to the desired necessary and sufficient criteria. Finally, for soliton systems there can exist a third method which, if known, is superior to the two mentioned before: the inverse scattering transform. It solves the initial-value problem directly and therefore can be used to answer all stability questions. However, there is no systematic way to construct the inverse scattering transform for an integrable system. That is the reason why we cannot use it here. In this paper we shall derive necessary and sufficient stability criteria for solitary-wave pulses in shape-memory alloys by Liapunov functionals and variational procedures.

The plan of the paper is as follows. In Sec. II. we shall discuss the model and the resulting equation of motion for the displacement of the atomic planes. The stationary solitary-wave solutions are discussed in Sec. III. There, we concentrate on pulse-type forms and show that solitons can exist in the austenitic as well as martensitic phase. Their explicit forms will be given either analytically or numerically. The stability even of the more general (and quite difficult) case, i.e., the soliton in the martensitic phase, will be treated in Sec. IV. From the constants of motion, a Liapunov functional is constructed and its definiteness properties are discussed. In those regions where it does not fulfill the requirements for a stability functional, variational principles for instability are developed. (In Appendix B, the simpler and analytically much easier case of a soliton in austenite is treated explicitly.) In Sec. V, the paper is concluded by a short discussion of the physical applications.

II. ONE-DIMENSIONAL MODEL AND EQUATION OF MOTION

In the one-dimensional model the crystal is built by stacking atomic planes parallel to the habit plane (Fig. 1).



FIG. 1. Sketch of the one-dimensional model.

The shear strain e, depending on time and position in stacking direction x, is in that plane in one direction only. Since the strain does not vary within each layer, the mass density remains constant. The displacement u(x,t) of the planes is related to the strain e by

$$e = \partial u / \partial x \equiv u_x \quad . \tag{2.1}$$

In a previous paper⁶ it was shown that, in reduced units, the Landau internal-energy density (Fig. 2).

$$U_L(e,S) = e^6 - e^4 + g(S)e^2 + U_0(S) ,$$

$$g(S) = -g_1 + g_2 \exp S, \quad U_0(S) = U_1 \exp S$$
(2.2)

describes the static behavior of homogeneously deformed shape-memory alloys. S is the entropy density and g_1, g_2 and U_1 are positive material parameters such that the monotonic function g(S) changes its sign in the entropy range of interest. Other material parameters are hidden in the rescaling of displacement, position, energy, entropy, and later on, time. For $g > \frac{1}{3}$ the internal energy has a single minimum at e = 0 representing the hightemperature-phase austenite, whereas for g < 0 there are just two symmetric minima representing two variants of the low-temperature-phase martensite. In the range $0 < g < \frac{1}{3}$, U_L shows three minima, that is, austenite and martensite are stable or metastable, reflecting the firstorder nature of the phase transition. In this way a single energy function describes all the phases involved.

Since we deal with situations where the strain is expected to vary strongly over short distances, an additional strain-gradient term has to be introduced into the internal energy density U:



FIG. 2. Landau internal energy $U_L(e)$ for different values of entropy parameter g $(-\frac{1}{16}, \frac{3}{16}, \frac{1}{4}, \frac{7}{24}, \frac{2}{5}, \text{ and } 1)$. U_0 is suppressed.

$$U(e, e_x, S) = U_L(e, S) + e_x^2 .$$
(2.3)

Because of symmetry and stability, the strain gradient gives, in lowest order, a positive quadratic contribution. The nonlinear shear stress $\sigma(e,S)$ is defined by

$$\sigma = \partial U / \partial e = \partial U_L / \partial e = 6e^5 - 4e^3 + 2g(S)e \quad . \tag{2.4}$$

In addition there is the couple stress

$$\mu(e_x) = \frac{\partial U}{\partial e_x} = 2e_x \quad . \tag{2.5}$$

In the following we deal with rapidly moving solitary waves, so we can neglect heat conduction. Neglecting also internal friction we end up with an adiabatic motion where the entropy remains constant. In the absence of external volume forces the equation of motion finally reads

$$\ddot{u} - \sigma_x + \mu_{xx} = 0 \quad . \tag{2.6}$$

Here we have to use expressions (2.1), (2.4), and (2.5) to understand Eq. (2.6) as a closed nonlinear partial differential equation for u(x,t). In addition, for an infinite crystal without external surface forces or surface moments, we assume the boundary values

$$\mu = 0 \quad \text{for } x \to \pm \infty \quad , \tag{2.7}$$

$$\sigma = 0 \quad \text{for } x \to \pm \infty \quad . \tag{2.8}$$

They induce the following boundary conditions (note $e = u_x$):

$$e_x = 0 \quad \text{for } x \to \pm \infty \quad .$$
 (2.9)

$$e = \begin{cases} e_{+\infty} & \text{for } x \to +\infty \\ e_{-\infty} & \text{for } x \to -\infty \end{cases},$$
(2.10)

where $e_{+\infty}$ and $e_{-\infty}$ are the strain values corresponding to the minima of U_L .

III. SOLITARY-WAVE SOLUTIONS OF PULSE-TYPE

Looking for solitary strain waves moving with constant velocity v, we make the ansatz

$$e(x,t) = e(x - vt) = e(z)$$
 (3.1)

which reduces the equation of motion (2.6) to the nonlinear ordinary differential equation

$$v^2 e_z - \sigma_z + \mu_{zz} = 0 . (3.2)$$

For a pulselike solitary wave the values of strain at $z = +\infty$ and at $z = -\infty$ are the same, i.e., in the boundary condition (2.10) we have

$$e_{+\infty} = e_{-\infty} = e_{\infty} \quad . \tag{3.3}$$

Integrating Eq. (3.2) yields after some rearrangements

$$z(e) = \int \frac{de}{\sqrt{R(e)}}$$
(3.4)

with

$$R(e) = U_L(e) - e^2 v^2 / 2 + v^2 e_{\infty} e + C . \qquad (3.5)$$

The constant of integration C is determined by the bound-

ary condition, which requires R(e) to have a double zero at e_{∞} [compare Eq. (3.3)].

The total energy of a solitary wave relative to its undisturbed value for the crystal is given by

$$E_{\text{tot}} = \int h(x,t)dx \quad , \tag{3.6}$$

where h is the Hamiltonian density

$$h = \dot{u}^2/2 + U(e,e_x) - U_L(e_\infty)$$
.

Due to the equation of motion for a pulselike solitary wave, kinetic energy density and strain-gradient energy density together equal just the Landau part of the energy density. Hence we have

$$h = \dot{u}^2 + 2e_x$$
.

Taking into account Eqs. (2.1) and (3.1) \dot{u} can be replaced by $-v(e-e_{\infty})$ if at $x = -\infty$ the crystal is at rest. Then the energy is given by

$$E_{\text{tot}}(v^2, g) = \int \left[v^2 (e - e_{\infty})^2 + 2e_z^2 \right] dz$$
(3.7)

with $e(z; v^2, g)$ and $e_{\infty}(g)$.

Because of energy conservation, E_{tot} does not depend on time. Remaining constant throughout the wave, the value of the entropy density may be calculated from the strain and the temperature T at infinity in front of the wave. T is given by

$$T = \partial U / \partial S = (dg / dS)e^2 + dU_0 / dS$$
$$= (g_2 e^2 + U_1) \exp S . \qquad (3.8)$$

A. Soliton in austenite

We assume the crystal to be in the austenitic phase with a moving solitary wave in it, which means $e_{\infty} = 0$. Because of symmetry the solitary wave can go to positive or negative strain; let us assume e > 0. The maximum amplitude e_m of the wave is given by that root of $R(e_m)=0$ which is closest to e = 0. Some algebra yields

$$e_m^2 = \left[1 - (2v^2 - 4g + 1)^{1/2}\right]/2 \tag{3.9}$$

or

$$v^2 = 2g - \frac{1}{2} + (1 - 2e_m^2)^2/2$$
 (3.10)

Hence the velocity of the wave is determined by its amplitude, which is restricted by

$$0 < e_m^2 < \frac{1}{2} - \sqrt{1/4 - g} \quad . \tag{3.11}$$

In a similar way we get from Eq. (3.11)

$$0 < v^2 < 2g$$
 . (3.12)

In the present case, the integral on the right-hand side of Eq. (3.4) can be evaluated and we obtain

$$e^{2}(z) = \frac{e_{m}^{2}}{1 + (1 - e_{m}^{2}/e_{1}^{2})\sinh^{2}(e_{1}e_{m}z)} , \qquad (3.13)$$

with

$$e_1^2 = 1 - e_m^2 > 0 \ . \tag{3.14}$$

Figures 3-5 show the dependence of the structure, velocity, and energy, respectively, of the soliton, on the amplitude. The soliton in austenite can, of course, only occur for g > 0 where there is an austenitic minimum in the internal energy. In the range $0 < g < \frac{1}{4}$, that is, if the austenitic minimum is higher than the martensitic ones, the soliton may occur even at rest with its highest amplitude possible. For very small amplitude⁶ the velocity approaches the acoustic wave velocity. The energy [see Eq. (3.6)] reads

$$E_{\text{tot}} = e_m e_1 / 2 + (v^2 + 2g - \frac{1}{2}) \operatorname{arctanh}(e_m / e_1)$$
. (3.15)

B. Soliton in martensite

In this case, the crystal is in the martensitic phase with a moving solitary wave in it. That means that e_{∞} is given by one of the martensitic minima of the internal energy, let us assume the right-hand minimum $(e_{\infty} > 0)$ with

$$e_{\infty}^{2} = (1 + \sqrt{1 - 3g})/3$$
 (3.16)

The amplitude of the soliton results from the lowest value e_m of the strain within the solitary wave, which is determined by the zero of R(e) closest to e_{∞} . Rather tedious algebra yields

$$v^{2} = 2(e_{m} + e_{\infty})^{2}(e_{m}^{2} - 1 + 2e_{\infty}^{2}) \ge 0.$$
(3.17)

This relation restricts e_m in the following way:

$$0 < (1 - 2e_{\infty}^{2})^{1/2} < e_{m} < e_{\infty} \quad \text{for } \frac{1}{4} < g < \frac{1}{3} , \qquad (3.18)$$

$$-e_{\infty} < e_m < e_2$$
 or $e_1 < e_m < e_{\infty}$ for $\frac{16}{75} < g < \frac{1}{4}$, (3.19)

$$-e_{\infty} < e_m < e_{\infty}$$
 for $g < \frac{16}{75}$. (3.20)

Here

$$e_1 = \left[-e_\infty + (8 - 15e_\infty^2)^{1/2} \right] / 4 , \qquad (3.21)$$

$$e_2 = -[e_{\infty} + e_1 - (-e_1 e_{\infty})^{1/2}] < e_1 < 0 .$$
 (3.22)

In the intermediate range of g there is not only an upper value of the amplitude but also a gap.

Unfortunately, here Eq. (3.4), determining the structure, and Eq. (3.6), determining the energy of the solitary



FIG. 3. Structure of the soliton in austenite e(x - vt) for different amplitudes. The profile depends only on the amplitude irrespective of temperature.



FIG. 4. Velocity of the soliton in austenite as a function of amplitude for different values of entropy parameter g. Below the dashed curve the waves are unstable.

wave, can be integrated only numerically. Examples of soliton structures are plotted in Fig. 6. Figure 7 shows the dependence of the wave velocity on the amplitude.

IV. STABILITY CRITERIA

In this section we investigate the stability behavior of the stationary (in a moving frame) pulselike solitary-wave solutions. We begin with a slight reformulation of the basic equations (2.6) and (3.2). The only reason for this modification is to bring the dynamical equations into some canonical form, which is more appropriate for standard stability considerations.

First, Eq. (2.6) can be written in the equivalent form (still in the laboratory frame)

$$u_{tt} + 2u_{xxxx} - \sigma'(u_x)u_{xx} = 0 , \qquad (4.1)$$

where the prime denotes the derivative with respect to the argument and the function $\sigma(u_x)$ is defined in Eq. (2.4).



FIG. 5. Energy of the soliton in austenite as a function of amplitude for different values of g. Below the lower dashed curve there is no solitary-wave solution. Between the dashed curves the solution is unstable.



FIG. 6. Structure of the soliton in martensite e(x - vt) for different amplitudes.

It is clear that Eq. (4.1) is the basic dynamical equation for all perturbations considered in this paper; the stability of the corresponding stationary (in a moving frame) solutions will be investigated in this paper. We shall use instead of e [as determined by Eq. (3.4), having, e.g., the form (3.13)]

$$G = e - e_{\infty} \quad . \tag{4.2}$$

Then G follows from Eq. (3.2), which we rewrite in the form

$$-G_{zz} + f(G) + \eta^2 G = 0 , \qquad (4.3)$$

where

$$f(G) = \frac{1}{2}\sigma(e_{\infty} + G) - \frac{1}{2}\sigma(e_{\infty})G , \qquad (4.4)$$

and

$$\eta^2 = \frac{1}{2}\sigma(e_{\infty}) - \frac{1}{2}v^2 .$$
(4.5)

In the two definitions of f and η^2 we have added and sub-



FIG. 7. Velocity of the soliton in martensite as a function of amplitude for different values of g. Outside the region limited by the dotted curves there is no soliton solution. Below the dashed curves the solution is unstable.

$$u_{tt} - 2vu_{zt} + v^2 u_{zz} + 2u_{zzzz} - \sigma'(u_z)u_{zz} = 0 .$$
 (4.6)

The boundary conditions can be easily translated from Eqs. (2.9) and (2.10):

$$u_z \to e_{\infty} \quad \text{for} \quad |z| \to \infty \quad , \tag{4.7}$$

$$u_{zz} \to 0 \quad \text{for} \quad |z| \to \infty$$
 (4.8)

and all finite times t. Then from Eq. (4.7), or the equivalent form $\sigma(u_z) \rightarrow 0$ for $|z| \rightarrow \pm \infty$ we also have

$$u_{zt} \to 0 \quad \text{for} \quad |z| \to \infty \quad .$$
 (4.9)

The latter condition allows only

$$u_t \to C_{\pm} \quad \text{for } z \to \pm \infty , \qquad (4.10)$$

where C_{\pm} are constants. Because of the Galilein invariance $(u \rightarrow u + \alpha t)$ we can choose, without loss of generality, the constants C_{\pm} in symmetric form, i.e.,

$$C_{\pm} = \pm K \quad . \tag{4.11}$$

Then it is straightforward to prove that Eq. (4.6) has (at least) two constants of motion. First, from the energy and momentum we construct

$$E = \int_{-\infty}^{+\infty} dz \left[\frac{1}{2} (u_{t}^{2} - K^{2}) + u_{zz}^{2} - \frac{v^{2}}{2} u_{z}^{2} + \frac{v^{2}}{2} e_{\infty}^{2} + v^{2} e_{\infty} (u_{z} - e_{\infty}) + U_{L} (u_{z}) - U_{L} (e_{\infty}) \right],$$

$$(4.12)$$

where $U_L'(u_x) = \sigma(u_x)$.

One finds

$$\frac{dE}{dt} = 2v \int_{-\infty}^{+\infty} dz \frac{d}{dz} (u_t^2 - K^2) = 0 .$$
 (4.13)

Secondly, for

$$Q = \int_{-\infty}^{+\infty} dz [u_{1}(u_{z} - e_{\infty}) - vu_{z}^{2} + ve_{\infty}^{2} + 2e_{\infty}v(u_{z} - e_{\infty})]$$
(4.14)

we obtain after some algebra

$$\frac{dQ}{dt} = \int_{-\infty}^{+\infty} dz \frac{d}{dz} [U_L(u_z) - U_L(e_\infty)] = 0 .$$
 (4.15)

The two constants of motion, E and Q, will play a key role in the stability analysis.

A. Liapunov functional for stability

We define the functional

$$L = E - E_s + \alpha^2 (Q - Q_s)^2 , \qquad (4.16)$$

where α^2 is a positive constant to be determined later.

The index s (on E and Q) should indicate that we evaluate the corresponding values [see Eqs. (4.12) and (4.14)] for $u = u_s(z - \xi)$, where $u_{sz}(z) - e_{\infty} = G$, as determined from Eq. (4.3). The shift parameter ξ allows us to take the socalled closest soliton as a reference state when stability with respect to form is considered. Still we have

$$\frac{dL}{dt} = 0 \tag{4.17}$$

although $\xi = \xi(t)$. The integrands in the constants of motion vanish for $z \rightarrow \pm \infty$ and the borders of integration do not change under the substitution $z \rightarrow z - \xi$.

Introducing the notation

$$\psi = u_t \quad , \tag{4.18}$$

$$\phi = u_z - e_{\infty} - G(z - \xi) = u_z - u_{zs} , \qquad (4.19)$$

we write

$$L = \delta L + \delta^2 L + \delta^{\ge 3} L \quad . \tag{4.20}$$

The first term on the right-hand side of Eq. (4.20) contains by definition the first-order contributions in ϕ and ψ ; the second term contains the second-order contributions, and so on. For δL we obtain

$$\delta L = 2 \int_{-\infty}^{+\infty} dz \,\phi [-G_{zz} + f(G) + \eta^2 G] = 0 , \qquad (4.21)$$

because of Eq. (4.3).

In the second order we have to deal with

$$\begin{split} \delta^{2}L &= \int_{-\infty}^{+\infty} dz \left[\frac{1}{2} \psi^{2} + \phi_{z}^{2} + \phi^{2} \left[-\frac{v^{2}}{2} + \frac{1}{2} \sigma' G + e_{\infty} \right] \right] , \\ &+ \alpha^{2} \left[\int_{-\infty}^{+\infty} dz \, \psi G - 2v \int_{-\infty}^{+\infty} dz \, \phi G \right]^{2} \\ &\equiv \frac{1}{2} \langle \psi \mid \psi \rangle + \langle \phi \mid H \mid \phi \rangle + \alpha^{2} (\langle \psi \mid G \rangle - 2v \langle \phi \mid G \rangle)^{2} . \end{split}$$

(4.22)

Here we have introduced the notation

$$\langle \cdots \rangle = \int_{-\infty}^{+\infty} dz \cdots$$
 (4.23)

and the operator

$$H = -\frac{d^2}{dz^2} + f'(G) + \eta^2 . \qquad (4.24)$$

H is a Schrödinger-type operator with the following properties:

$$HG_z = 0 , \qquad (4.25)$$

$$H^{-1}G = -G_{\eta^2} \equiv -\frac{\partial}{\partial \eta^2}G \quad . \tag{4.26}$$

Since G is pulselike, and thus G_z has a node, the Schrödinger-type operator possesses an eigenfunction e_{-} with a negative eigenvalue λ_{-} . In Appendix A we shall derive the auxiliary estimates

$$\frac{1}{2} \langle \psi | \psi \rangle + \alpha^{2} (\langle \psi | G \rangle - 2v \langle \phi | G \rangle)^{2}$$

$$\geq 2(1 - \chi \epsilon) v^{2} \langle \phi | G \rangle^{2} \langle G | G \rangle^{-1} + \frac{1}{2} \epsilon \langle \psi | \psi \rangle \qquad (4.27)$$

for sufficiently small $\epsilon > 0$, $\chi > 1$, $\epsilon \chi \ll 1$, and $\alpha^2 \epsilon \gg 1$.

Furthermore, to estimate the remaining term $\langle \phi | H | \phi \rangle$ in $\delta^2 L$, we also prove in Appendix A that for

$$\langle G | H^{-1} | G \rangle < 0 \tag{4.28}$$

and even functions a with

$$\langle a \mid G \rangle = 0 , \qquad (4.29)$$

$$\langle a \mid H \mid a \rangle > 0 \tag{4.30}$$

holds. Finally, we prove in Appendix A that under the condition (4.28), but with $\langle a | G \rangle \neq 0$, the estimate

$$\langle a \mid H \mid a \rangle \ge \langle G \mid H^{-1} \mid G \rangle^{-1} \langle a \mid G \rangle^{2}$$
(4.31)

holds for even functions a.

Using the results (4.27), (4.30), and (4.31) we can draw the following conclusions.

(i) The odd parts (b) of ϕ make $\delta^2 L$ positive since the translation mode $\phi = G_z$ can be excluded by the argument that we are considering stability with respect to form.

(ii) The even parts (a) of ϕ lead to sufficient stability criteria when we calculate the sign of $\delta^2 L$.

(iii) A sufficient criterion for stability is that under the condition (4.28)

$$\langle G | H^{-1} | G \rangle^{-1} + 2v^2 \langle G | G \rangle^{-1} > 0$$
(4.32)

holds.

(iv) Because of relation (4.26) we can rewrite the sufficient criteria for stability in the simplest form

$$\frac{\partial}{\partial \eta^2} \langle G \mid G \rangle > 0 , \qquad (4.33)$$

and

$$v^{2} \frac{\partial}{\partial \eta^{2}} \langle G \mid G \rangle > \langle G \mid G \rangle , \qquad (4.34)$$

where $\langle G | G \rangle$ depends on η and g.

Note that now the criterion (4.34) alone is sufficient as it stands. From Eq. (4.5) it follows that the derivative $\partial/\partial \eta^2$ may be replaced by $-2\partial/\partial v^2$, with g and therefore e_{∞} fixed. By a straightforward calculation it can be shown from Eq. (3.7) that inequality (4.34) is equivalent to

$$\frac{\partial E_{\rm tot}(v^2,g)}{\partial v^2} < 0 \; .$$

Since the velocity v of the soliton is monotonically decreasing with its amplitude Δe (Figs. 4 and 7), the stability condition may instead be written

$$\frac{\partial E_{\rm tot}(\Delta e,g)}{\partial \Delta e} > 0 \; .$$

So the soliton is stable if its energy increases with amplitude.

(v) For small but finite perturbations the sign of $\delta^2 L$ will determine the sign of L; therefore physically it seems reasonable to abandon the discussion of $\delta^{\geq 3}L$. Mathematically, the estimate of $\delta^{\geq 3}L$ can be performed by making use of the Sobolev inequalities.

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B. A variational principle for instability

In this subsection we want to show that in the region complementary to (4.34) instability occurs. For that purpose we use a method which has been proved already to be successful in many soliton systems.¹⁰

Remember that the basic equation determining the dynamical behavior of our system is Eq. (4.6). When linearizing it with respect to the soliton solution and using the notation (4.19), we arrive at

$$\phi_{tt} - 2v\phi_{tz} - 2\partial_z H \partial_z \phi = 0 \tag{4.35}$$

for the perturbations ϕ . Motivated by the search for an exponential instability $[\phi \sim \exp(\gamma t)]$, we investigate first a related model system, where part of the time derivatives have been simplified by assuming already a time dependence of the form $\sim \exp(\delta t)$. (Later on, we shall set $\gamma = \delta$.) The model system in mind is

$$v\psi_t = -\partial_z \mathcal{H}\psi \tag{4.36}$$

with

$$\mathcal{H} = H - \frac{\delta}{2} \partial_z^{-2} . \tag{4.37}$$

If we split ψ into its odd (u) and even (g) contributions

$$\psi = g + u \quad , \tag{4.38}$$

and define

$$h(\delta^{2}) = \frac{1}{v^{2}} \sup_{u} \left\{ \frac{-\langle u | -\partial_{z} \mathcal{H} \partial_{z} | u \rangle}{\langle u | \mathcal{H}^{-1} | u \rangle} \right\}$$
(4.39)

(where \mathcal{H} is positive for odd functions), then the exponential growth rate γ of the system (4.37) is given by¹¹

$$\gamma^2 = h(\delta^2) . \tag{4.40}$$

In Eq. (4.39), the supremum has to be evaluated for all odd test functions u. It has been further shown¹⁰ that the original system (4.35) is unstable with a growth rate γ if the implicit equation

$$\gamma^2 = h(\gamma^2) \tag{4.41}$$

possesses a positive solution. Thus the rest of this subsection is devoted to the proof that Eq. (4.41) has a positive solution in the region complementary to (4.34). The general procedure is as follows. One can show¹⁰ that

$$\lim_{\delta^2 \to \infty} h(\delta^2) = 0 .$$
(4.42)

Then by continuity arguments, instability will follow if we can show (by chosing appropriate test functions) that h(0) > 0 or $h(\delta) \sim c\delta^{\nu}$ for $\delta \ll 1$, with a factor c and an exponent ν such that a solution of Eq. (4.41) exists. Let us briefly summarize the results for the following cases

(I)
$$\langle G | H^{-1} | G \rangle > 0$$
. (4.43)

The localized integral form of

i.e.,

$$f = \langle G | G \rangle H^{-1}G - \langle G | H^{-1} | G \rangle G , \qquad (4.44)$$

$$\widetilde{u} = \int_0^z [f(\xi) - \epsilon f(\epsilon \xi)] d\xi \qquad (4.45)$$

for $\epsilon \rightarrow 0$, can be used to construct a test function with the intended result. The function

$$u = \langle G_z | G_z \rangle \tilde{u} + \langle \tilde{u}_z | G \rangle G_z$$
(4.46)

has the property

$$\langle u \mid G_z \rangle = 0 , \qquad (4.47)$$

which guarantees that $H^{-1}u$ exists. Some simple calculations yield

$$u_{z} = \langle G_{z} | G_{z} \rangle f(z) - \epsilon \langle G_{z} | G_{z} \rangle f(\epsilon z) - \epsilon \langle f(\epsilon z) | G \rangle G_{zz} .$$
(4.48)

When using this in the numerator on the right-hand side of Eq. (4.39) for $\delta = 0$, i.e., when calculating

$$-\langle u_{z} | H | u_{z} \rangle = \langle G_{z} | G_{z} \rangle^{2} (\langle G | G \rangle^{2} \langle G | H^{-1} | G \rangle$$
$$-\langle G | H^{-1} | G \rangle^{2} \langle G | H | G \rangle)$$
$$+ O(\epsilon) , \qquad (4.49)$$

we can determine the sign of the right-hand side of Eq. (4.49). Namely, in the case (I), Eq. (4.43), we get

$$-\langle u_z | H | u_z \rangle > 0 , \qquad (4.50)$$

since $\langle G | H | G \rangle < 0$ and thereby

$$h(\delta^2 = 0) > 0$$
, (4.51)

implying instability.

The second case is

$$(II) \quad \langle G \mid H^{-1} \mid G \rangle < 0 ; \qquad (4.52)$$

then a calculation analogous to the first case can be performed. Let us choose

$$f = H^{-1}G (4.53)$$

and the same definition (4.45) for the localized integral form of f. In Appendix C we shall show then that for $0 < \delta \ll 1$ the estimate

$$h(\delta^2) \ge -\frac{\delta^2}{2v^2} \frac{\langle G \mid G \rangle}{\langle G \mid H^{-1} \mid G \rangle} [1 + O(\delta^{1/2})] \qquad (4.54)$$

holds. This clearly shows that under the condition (4.52) and for

$$\langle G | H^{-1} | G \rangle^{-1} + 2v^2 \langle G | G \rangle^{-1} < 0$$
, (4.55)

a positive solution of Eq. (4.41) is possible. The reason is that for (4.55), $h(\delta^2)$ first grows faster than δ^2 for $0 < \delta^2 \ll 1$, but from Eq. (4.42) we know that this behavior will change later so that instability is possible. Note that condition (4.55) is complementary to (4.32).

The final case is

(III)
$$\langle G | H^{-1} | G \rangle = 0$$
. (4.56)

The corresponding argument parallels over a wide range that in the second case (II) when we use

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$$u = \int_{0}^{z} d\xi [f(\xi) - \epsilon f(\epsilon \xi)] + \delta^{1/4} \int_{0}^{z} d\xi [G(\xi) - \epsilon G(\epsilon \xi)]$$
(4.57)

as a test function. The final result is

$$h(\delta^2) \sim \delta \tag{4.58}$$

for $0 < \delta \ll 1$, and this again clearly shows that instability is possible.

We have thereby arrived at the final conclusion: The stability conditions as summarized in the formulas (4.33) and (4.34) are sufficient and necessary. We renounce a possible calculation of the maximum growth rates γ in the unstable region. The regions of instability are marked in the corresponding Figs. 3, 4, and 6.

V. SUMMARY AND CONCLUSIONS

Within the framework of a one-dimensional Ginzburg-Landau theory for the martensitic phase transition it was shown that in martensite as well as in austenite there exist solitary-wave solutions of the pulse type for the shear strain. In both the cases the velocity of the wave decreases with increasing amplitude; even a static solution exists. Static solutions, as well as slowly moving ones, are unstable in form with respect to perturbations of the initial conditions. Hence the static solution represents the critical nucleus. In this paper we did not investigate the mode of highest growing rate. Nevertheless, a simple calculation shows that a pulse a little bit smaller than the unstable critical nucleus has lower potential energy, that is, it further shrinks. On the other hand, a pulse a little bigger than the critical one has lower energy too, hence it will further grow. Thus the static critical nucleus is unstable in both directions. Using numerical values for the parameters involved, e.g., as determined for AuCuZn₂ in a previous paper,⁶ the energy of the static critical nucleus in both cases, martensitic or austenitic nucleus, referring to the cross-sectional area perpendicular to the stacking direction, if of the order of magnitude of 0.1 eV/nm^2 . The same value applies to moving pulses for not-too-small amplitudes. The energy mentioned is a result of the onedimensional model. Therefore contributions due to elastic misfit in the plane perpendicular to the stacking direction are not included. These contributions, however, are proportional to the diameter of the nucleus; that is, they grow with the square root of the cross-sectional area only.

It was further shown that pulselike solitary waves are stable if moving faster than some threshold speed, which in turn is lower than the acoustic wave velocity. In the present paper, the initial-value problem for the nonlinear equations of motion was not solved. This can be done only numerically.

The current forecasted picture, however, is that soliton will propagate with unchanging profile in a stable manner. It may be assumed that initial data near that of the soliton will produce a soliton plus phonons. Therefore it is reasonable to predict that a moving soliton can be emitted by a pulselike shearing force on the surface, even if its time profile does not exactly meet the profile of the soliton to be generated. In this way nuclei can be transmitted through a crystal. For example, imagine a polycrystal where one grain undergoes a phase transition from austenite to martensite after a heterogeneous nucleation process. When the phase boundary reaches the grain boundary there is a jumping surface force exerted on the neighboring grain where a stable pulselike soliton may be generated if temperature and local static stress are favorable. A soliton emitted into the untransformed grain with a temperature gradient in it may run into a region of slightly different temperature where the soliton becomes unstable, thus representing a critical nucleus which can initiate the phase transition in the grain. This may happen even if the force on the surface was not high enough to trigger the phase transition directly. Another possibility for the previously stable soliton to become unstable is to run into a stress concentration generated, e.g., by a dislocation. A stress field reduces the local value of the shear modulus which is represented by the parameter g. Therefore the stress concentration influences the stability of solitons in a similar way as temperature does. As a result dislocations may serve as soliton-assisted nucleation centers even if their own nucleation potency is not sufficient to start the phase transition. Based on these considerations it is proposed that stable pulselike solitary waves are important as a new mechanism for autocatalytic nucleation processes¹² in shape-memory alloys.

APPENDIX A: SOME USEFUL ESTIMATES

First we prove the relation (4.27). The Schwarzs inequality yields

$$\langle \psi | \psi \rangle \ge \langle \psi | G \rangle^2 \langle G | G \rangle^{-1}$$
 (A1)

We write

$$\frac{1}{2} \langle \psi | \psi \rangle \ge \frac{\epsilon}{2} \langle \psi | \psi \rangle + \frac{1 - \epsilon}{2} \frac{1}{\langle G | G \rangle} \langle \psi | G \rangle^2 , \qquad (A2)$$

where ϵ is some sufficiently small positive number to be determined later. Using this on the left-hand side of inequality (4.27), we obtain, after some algebraic manipulations,

$$\frac{1}{2}\langle\psi|\psi\rangle + \alpha^{2}(\langle\psi|G\rangle - 2v\langle\phi|G\rangle)^{2} \geq \left[\alpha^{2} + \frac{1-\epsilon}{2}\frac{1}{\langle G|G\rangle}\right]\langle\psi|G\rangle^{2} - 4\alpha^{2}v\langle\psi|G\rangle\langle\phi|G\rangle + 4\alpha^{2}v^{2}\langle\phi|G\rangle^{2} + \frac{\epsilon}{2}\langle\psi|\psi\rangle$$

$$\geq \frac{2v^2}{\langle G | G \rangle} \frac{(1-\epsilon)\alpha^2}{\alpha^2 + \frac{1-\epsilon}{2} \frac{1}{\langle G | G \rangle}} \langle \phi | G \rangle^2 + \frac{\epsilon}{2} \langle \psi | \psi \rangle .$$
(A3)

Thus for

$$(\chi - 1)\epsilon \alpha^2 \ge (1 - \epsilon)(1 - \chi \epsilon) / (2\langle G \mid G \rangle) , \qquad (A4)$$

which can be fulfilled for sufficiently large α^2 , small ϵ , and $\chi > 1$, the estimation (4.27) follows. Take for example $\alpha \sim \epsilon^{-1}$ and χ fixed for $\alpha \to \infty$.

Next we derive (4.30). Any even function a we can decompose into a component parallel to e_{-} and the rest being perpendicular to e_{-} , i.e.,

$$a = \frac{\langle a \mid e_{-} \rangle}{\langle e_{-} \mid e_{-} \rangle} e_{-} + a_{\perp} = a_{-} + a_{\perp} .$$
 (A5)

Then we have

$$\langle a | H | a \rangle = - | \lambda_{-} | \langle a_{-} | a_{-} \rangle + \langle a_{\perp} | H | a_{\perp} \rangle$$
 (A6)

Because of
$$\langle a | G \rangle = 0$$
, Eq. (4.29), we can derive for

$$F = H^{-1}G \tag{A7}$$

the helpful relation

$$- |\lambda_{-}| \langle a_{-}|F_{-}\rangle + \langle a_{\perp}|H|F_{\perp}\rangle = 0 , \qquad (A8)$$

which can be used in the Schwarz inequality

$$\langle a_{\perp} | H | a_{\perp} \rangle \geq \langle a_{\perp} | H | F_{\perp} \rangle^{2} \langle F_{\perp} | H | F_{\perp} \rangle^{-1}$$

$$\geq | \lambda_{-} |^{2} \langle a_{-} | F_{-} \rangle^{2} \langle F_{\perp} | H | F_{\perp} \rangle^{-1} .$$
(A9)

Thus, we can transform Eq. (A6) into the form

$$\langle a | H | a \rangle \geq - |\lambda_{-}| \langle a_{-} | a_{-} \rangle + |\lambda_{-}|^{2} \langle a_{-} | a_{-} \rangle \langle F_{-} | F_{-} \rangle \langle F_{\perp}| H | F_{\perp} \rangle^{-1}$$

$$\geq |\lambda_{-}| \langle a_{-} | a_{-} \rangle \langle F_{\perp}| H | F_{\perp} \rangle^{-1} (-\langle F | H | F \rangle) .$$
(A10)

For $\langle F | H | F \rangle < 0$, Eq. (4.28), we therefore get the desired result (4.30) since H is positive definite in the function space orthogonal to e_{-} and G_{z} .

Finally we present the relevant arguments for the estimate (4.31). Let us discuss for that purpose

$$i = \inf_{\substack{\xi \text{ even}}} \left\{ \frac{\langle \xi | H | \xi \rangle}{\langle \xi | G \rangle^2} \right\},$$
(A11)

i.e., the infimum of the right-hand side of (A11) when varied over all possible even test functions ξ , which exists because of the foregoing arguments. We replace in the denominator on the right-hand side of Eq. (A11) $\langle \xi | G \rangle^2$ by $\langle \xi | H | F \rangle^2$ and introduce instead of the test functions ξ ,

$$\delta = \xi - F , \qquad (A12)$$

with the normalization

$$\langle F + \delta | H | F \rangle = \langle F | H | F \rangle$$
 (A13)

Then the definition (A11) reads

$$i = \inf_{\substack{\delta \text{ even}}} \left\{ \frac{\langle F \mid H \mid F \rangle + \langle \delta \mid H \mid \delta \rangle}{\langle F \mid H \mid F \rangle^2} \right\}$$
$$= \langle F \mid H \mid F \rangle^{-1} .$$
(A14)

Combining the statements contained in (A11) and (A14), it is straightforward to draw the conclusion (4.31).

APPENDIX B: STABILITY OF A SOLITON IN AUSTENITE

In this appendix we rederive the stability criterion for a soliton in austenite although all the calculations of Sec. IV do apply for this special case. The reason is that (i) we can easily show the similarity to the so-called Q stability,⁹ and (ii) the stability criteria (4.33) and (4.34) can be evaluated explicitly.

In the present case $(e_{\infty}=0)$ we use $E-E_s$ itself as a Liapunov functional and vary for $\delta Q=0$ (Q stability). The first variation vanishes because of the stationary equation (4.3) and for the second variation we obtain

$$\delta^2 E = \int_{-\infty}^{+\infty} dz \left(\frac{1}{2} \phi_t^2 + \phi_z H \phi_z \right) , \qquad (B1)$$

where

$$H = -\frac{d^2}{dz^2} + \frac{1}{2}\sigma'(G) - \frac{1}{2}v^2 , \qquad (B2)$$

when

$$\phi = u - u_s \quad , \tag{B3}$$

and

$$G = u_{sz} \quad . \tag{B4}$$

The subsidiary condition $\delta Q = 0$ implies

$$\int_{-\infty}^{+\infty} dz \,\phi_t G = 2v \,\int_{-\infty}^{+\infty} dz \,\phi_z G \,. \tag{B5}$$

By the Schwarz inequality

$$\left(\int_{-\infty}^{+\infty} dz \,\phi_t^2\right) \left(\int_{-\infty}^{+\infty} dz \,G^2\right) \geq \left(\int_{-\infty}^{+\infty} dz \,\phi_t G\right)^2;$$
(B6)

we then obtain from (B1)

$$\delta^{2}E \geq 2v^{2}\langle G \mid G \rangle^{-1}\langle \phi_{z} \mid G \rangle^{2} + \langle \phi_{z} \mid H \mid \phi_{z} \rangle , \quad (\mathbf{B7})$$

when use is made of Eq. (B5). Introducing

$$\psi = \phi_z \tag{B8}$$

we rewrite (B7) in the form

$$\delta^{2}E \geq \langle G \mid G \rangle^{-1} \langle \psi \mid G \rangle^{2} \left[2v^{2} + \frac{\langle \psi \mid H \mid \psi \rangle}{\langle \psi \mid G \rangle^{2}} \langle G \mid G \rangle \right].$$
(B9)

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The estimate (4.31) now immediately leads to the stability condition (4.32), together with (4.28).

With the abbreviation

$$N = \langle G \mid G \rangle \tag{B10}$$

and $\eta^2 = -\frac{1}{2}v^2$, the stability condition (4.32) can be written as

$$\frac{d}{dv}(Nv) < 0 . (B11)$$

For the solution (3.13) we have

$$N = \int_{-\infty}^{+\infty} dz \frac{q}{1 + (1 - q^2) \sinh^2 z} = 2 \operatorname{arctanh} q \qquad (B12)$$

and

$$v^2 = 2g - \frac{1}{2} + \frac{1}{2} \left(\frac{1-q}{1+q} \right)^{1/2}$$
, (B13)

where

 $q = e_m / e_1$.

For the explicit evaluation we can use instead of criterion (B11),

$$\frac{2g - \frac{1}{2} + \frac{1}{2} \left(\frac{1-q}{1+q}\right)^{1/2}}{\left[(1-q)(1+q)\right]^{1/2}} \frac{dN}{dq} > N , \qquad (B14)$$

which reads

$$g > e_m^2 e_1^2 + e_m e_1 (e_1^2 - e_m^2)^2 \operatorname{arctanh}(e_m / e_1)$$
. (B15)

The results are introduced in Figs. 4 and 5.

APPENDIX C: INVESTIGATION OF THE INSTABILITY REGION (4.55)

In this Appendix, we treat the second case (II) [see Eq. (4.52)] in more detail, i.e., we prove the estimate (4.54). With that intention, we calculate the numerator

$$Z = -\langle u_z | \mathcal{H} | u_z \rangle \tag{C1}$$

and the denominator

$$N = \langle u \mid \mathcal{H}^{-1} \mid u \rangle , \qquad (C2)$$

appearing on the right-hand side of Eq. (4.39) for some test function in the case $0 < \delta \ll 1$. Inserting the function (4.53) into the definition (4.45) we obtain

$$u = \int_{0}^{z} d\xi [H^{-1}G(\xi) - \epsilon H^{-1}G(\epsilon\xi)] .$$
 (C3)

Straightforward evaluation of Z yields

$$Z = -\langle G | H^{-1} | G \rangle + \frac{\delta^2}{2} \langle u | u \rangle + O(\epsilon) .$$
 (C4)

One should note that

$$\langle u \mid u \rangle = O(1/\epsilon)$$
 (C5)

Therefore we choose $\epsilon = \delta^{\beta}$ with $\beta > \frac{1}{2}$ to obtain from Eq. (C4)

$$Z = -\langle G | H^{-1} | G \rangle + O(\delta^{\beta}, \delta^{2-\beta}) .$$
 (C6)

Next we calculate N. When doing this we formally rewrite u, i.e.,

$$u = \alpha F + u_{\perp} , \qquad (C7)$$

where $\langle u_{\perp} | G_z \rangle = 0$ by definition and the (yet undetermined) function F should have a component parallel to G_z . Then the coefficient α is

$$\alpha = \langle u \mid G_z \rangle \langle F \mid G_z \rangle^{-1} . \tag{C8}$$

Using the Schwarz inequality, we find for odd functions (u) with the positive-definite operator \mathcal{H}^{-1} (for $0 < \delta$),

$$N \leq \alpha^{2} \langle F | \mathcal{H}^{-1} | F \rangle$$

+ 2\alpha \langle F | \mathcal{H}^{-1} | F \rangle^{1/2} \langle u_{\perp} | \mathcal{H}^{-1} | u_{\perp} \rangle^{1/2}
+ \langle u_{\perp} | \mathcal{H}^{-1} | u_{\perp} \rangle . (C9)

Estimating the terms appearing on the right-hand side of inequality (C9), one has

and

$$\langle u_{\perp} | \mathcal{H}^{-1} | u_{\perp} \rangle \leq \langle u_{\perp} | H^{-1} | u_{\perp} \rangle$$

$$\leq \eta^{-2} \langle u_{\perp} | u_{\perp} \rangle \leq \eta^{-2} \langle u | u \rangle \sim O(1/\epsilon) .$$
(C11)

Now we can simplify (C9):

$$N \leq \frac{2}{\delta^2} \langle u_z \mid G \rangle^2 \langle F_z \mid G \rangle^{-2} \langle F_z \mid F_z \rangle + O(\delta^{-(2+\beta)/2}) .$$
(C12)

The choice

$$F = \int_{0}^{z} d\xi [G(\xi) - \epsilon G(\epsilon \xi)]$$
(C13)

leads to

$$N \leq \frac{2}{\delta^2} \langle G \mid H^{-1} \mid G \rangle^2 \langle G \mid G \rangle^{-1} + O(\delta^{-(2+\beta)/2}, \delta^{-\beta}) .$$
(C14)

For $\beta = 1$, the use of the estimates (C6) and (C14) immediately leads to (4.54) for $0 < \delta^2 \ll 1$.

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