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LETTER TO THE EDITOR

Dynamical behaviour of interacting twin boundaries in martensitic transformations

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Abstract. We study the dynamics of interacting twin boundaries in martensites on the basis of the one-dimensional continuum model. Applying the method recently developed by Kawasaki to the model, we derive for the first time the equation of motion of twin boundaries. The equation obtained is found to be more advantageous than the original model for considering the dynamical behaviour of twin boundaries.

The dynamics of coherent alternating twins or domain structures are of considerable interest in structural and martensitic phase transitions [1, 2]. The coexistence of a few distinct variants or twins of the product phase, formed within the parent phase, results in localised twin boundaries. It has been shown [3–5] that static solutions for a twin boundary (TB) and for a periodic array of TBs can be produced entirely in the framework of the Ginzburg–Landau-type model. Moreover, Falk has extended the model to the time-dependent one and obtained the solitary wave solution for the TB with stationary periodic shape and constant velocity [6].

These authors have, however, discussed only ideal solutions that describe a regular or periodic array of TBs. In the present Letter we thus consider a general situation where the positions of the TB are randomly arranged. By making use of virtual changes in the TBs, we reduce the equation of motion of the TBs from the one-dimensional Ginzburg–Landau-type model [4]. This method has been developed by Kawasaki for various topological singularities (e.g. domain walls and vortex lines) [7].

Recently Barsch and co-workers [8, 9] have discussed the formation of a periodic twinning array. In order to stabilise such periodic TBs, they have considered the long-range interactions between the TBs mediated via the parent phase. The present work is in some manner complementary to that of Barsch and co-workers in the sense that we are concerned with very slow motion of the TBs, after almost completing their formations, due to short-range and weak interactions between the TBs. Such a process is known to be important in the late stage dynamics [7].

Consider an array of TBs parallel to the (110) plane. This structure may be described by an elastic displacement field $u(x, t)$ in the $[1\bar{1}0]$ direction and an associated shear-strain field $e(x, t)$ defined by

$$e(x, t) = (\partial/\partial x)u(x, t) \tag{1}$$

where x is in the [110] direction and t the time. The TBs in martensitic phase transitions

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of Cu–Zn, Ag–Cd and Ni–Al alloy systems have such a structure [1, 2]. Following the notations of Falk [4], the equation of motion for the system is rewritten as

$$\ddot{u}(x, t) = (\partial/\partial x)[-2(\partial^2/\partial x^2)e + (\delta/\delta e)f(e, T)] \tag{2}$$

where a dot denotes the time derivative, T the temperature, and $f(e, T)$ the Landau free energy density defined by

$$f(e, T) = e^6 - e^4 + (T + \tfrac{1}{4})e^2. \tag{3}$$

Note that all the above quantities are expressed in suitably rescaled units. Note also that here we have neglected external forces and friction effects. It is shown [4] that in this model a twin boundary solution can be obtained for $T < 0$. In fact, an isolated static TB solution between martensitic domains $\pm e_m$ (called a kink solution) is given by

$$e_i(x) = e_m \sinh[(x - x_i)/z]\{C + \sinh^2[(x - x_i)/z]\}^{-1/2} \tag{4}$$

$$e_m(T) = [1 + (1 - 12T)^{1/2}/2]^{1/2}/\sqrt{3} \tag{5}$$

$$C(T) = (3e_m^2 - 1)/(2e_m^2 - 1) \tag{6}$$

$$1/z(T) = e_m(2e_m^2 - 1)^{1/2} \tag{7}$$

where x_i denotes the twin boundary position and $z(T)$ the twin boundary thickness, assumed to be sufficiently small.

In the presence of many kinks or twin boundaries, as is shown in figure 1, superposition of an isolated static TB solution (4) is no longer stationary, but the TBs start to move due to interactions between the TBs. Hereafter positions of the TBs are numbered consecutively from left to right along the x axis. To include effects of neighbouring TBs for the ith TB, the profile of $e(x, t)$ near x_i is approximated by [7]

$$e(x, t) = e_i(x) + \sum_{j>i} [e_j(x) - e_j(-\infty)] + \sum_{j<i} [e_j(x) - e_j(+\infty)]. \tag{8}$$

Differentiating (2) with respect to x and using (1) and (8), we find

$$\sum_j [-\ddot{x}_j e_j' + \dot{x}_j^2 e_j''] = (\partial^2/\partial x^2)[-2e_{xx} + f'(e, T)] \tag{9}$$

where the primes denote differentiation and $e_{xx} = (\partial^2/\partial x^2)e$. Introducing the one-dimensional Green function

$$G(x, x') = -|x - x'|/2 \tag{10}$$

which satisfies $(\partial^2/\partial x^2)G(x, x') = -\delta(x - x')$, (9) is written as

$$\sum_j \int_{-\infty}^{+\infty} \mathrm{d}x'\, G(x, x')(-\ddot{x}_j e_j'(x') + \dot{x}_j^2 e_j''(x')) = 2e_{xx} - f'(e, T). \tag{11}$$

Here we have ignored the arbitrary function $A(x)$ which satisfies $(\partial^2/\partial x^2)A(x) = 0$ by

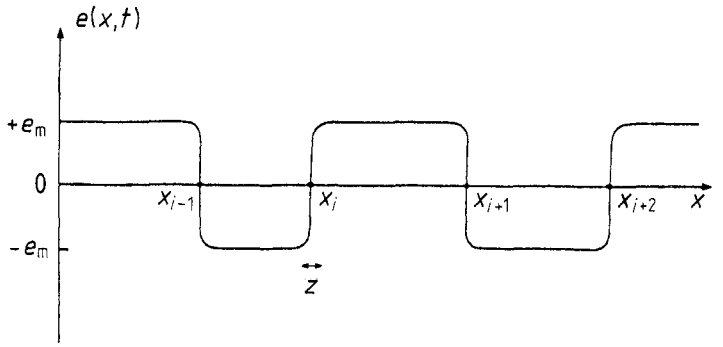

Figure 1. The strain field profile $e(x, t)$ for the one-dimensional case. The thickness of twin boundaries is $z(T)$.

way of an approximation. Contributions of this function $A(x)$ to the following result will be discussed elsewhere [10]. We integrate (11) over x after multiplying by $e_i'(x)$

$$\sum_j (-\langle e_i', e_j'\rangle \ddot{x}_j + \langle e_i', e_j''\rangle \dot{x}_j^2) = \int_{-\infty}^{+\infty} \mathrm{d}x\, e_i' [2e_{xx} - f'(e, T)] \tag{12}$$

with

$$\langle A, B\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}x'\, A(x)B(x'). \tag{13}$$

Moreover, using equations (1), (2) and (8) and integrating by parts, as well as $[2(\partial^2/\partial x^2) - f''(e_j, T)]e_j' = 0$, the right-hand side of (12) becomes

$$-\langle e_i', \Delta f_i\rangle \tag{14}$$

with

$$\Delta f_i = f'(e, T) - f'(e_i, T) - \Delta e_i f''(e_i, T) \tag{15}$$

$$\Delta e_i = e(x, t) - e_i(x). \tag{16}$$

If the interactions are limited to be between adjoining TB pairs, (14) becomes a simple form as follows:

$$\langle e_i', \Delta f_i\rangle = R(x_{i+1} - x_i) - R(x_i - x_{i-1}) \tag{17}$$

with

$$R(x_i - x_j) = -D(T)[e_j(x_i) - e_m] \tag{18}$$

$$D(T) = 16e_m(e_m^2 - T - \tfrac{1}{4}). \tag{19}$$

Thus we have the equation of motion for the TB position

$$\sum_j (\langle e_i', e_j'\rangle \ddot{x}_i - \langle e_i', e_j''\rangle \dot{x}_j^2) = R(x_{i+1} - x_i) - R(x_i - x_{i-1}) \tag{20}$$

where the driving force is the short-range interactions between adjoining TB pairs represented by the right-hand side of (20). To discuss the dynamical behaviour of TB,

(20) is more advantageous than (2). This is because (20) reduces the structure of the TBS to an assembly of the positions of TBS with an enormous reduction of information [7].

The above equation of motion (20) is, however, still difficult to handle. A considerable simplification is obtained if $|x_{i+1} - x_i|/z \gg 1$. In this limiting case we obtain

$$R(x) = D(T)(2C(T) + 1)e_m \exp(-2x/z) \tag{21}$$

$$\langle e_i' , e_j' \rangle = 2(-1)^{i-j+1} e_m^2 |x_i - x_j| \tag{22}$$

$$\langle e_i' , e_j'' \rangle = 0. \tag{23}$$

Then (20) reduces to

$$\sum_j (-1)^{i-j+1} |x_i - x_j| \ddot{x}_j = g\{\exp[-2(x_{i+1} - x_i)/z] - \exp[-2(x_i - x_{i-1})/z]\} \tag{24}$$

with

$$g = 8(e_m^2 - T - \tfrac{1}{4})(2C(T) + 1). \tag{25}$$

To discuss a deviation from the above simplification, we are now performing molecular dynamics simulations of (20) directly. The result, together with further details of the derivation of (20), as well as the relation between the present result and that of Barsch and co-workers, will be published in the future [10].

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