On the velocity of twin boundary

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Abstract The velocity of twin boundaries is estimated in the framework of continuum mechanics using the internal variables approach. It is shown that the slow motion of twin boundaries can be reproduced using a single internal variable. To comprehend the fast dynamics of twin boundaries, the concept of dual internal variables is employed.

1 Introduction

Twin boundary velocity is a macroscopic characteristic of the twinning process. The velocity is measurable, but experimental results range from near-zero up to sound velocity of a material.

Despite differences in experimental settings, there is evidence of rapid twin tip propagation (Takeuchi, 1966; Williams and Reid, 1971; Mahajan and Williams, 1973; Reed-Hill et al., 1973; Kannan et al., 2018). At the same time, various researchers have reported moderate twin boundary velocities ranging from 30 to 300 m/s (Bowden and Cooper, 1962; Smith et al., 2014; Saren et al., 2016, 2023). Even smaller values (from 0 to 14 m/s) for the velocity of the twin boundary were experimentally recorded recently (Mizrahi et al., 2020; Shilo et al., 2021). It is desirable that the scatter of the macroscopic quantity be described in terms of continuum mechanics.

There have been numerous theoretical and computational studies conducted on twin boundary motion. In phase field models (Hu et al., 2010; Levitas et al., 2013; Grilli et al., 2020; Amirian et al., 2022, c.f.), crystal plasticity models (Mirkhani and Joshi, 2014, e.g.), or combinations thereof (Liu et al., 2018; Rezaee-Hajidehi et al., 2022) individual twin boundaries are not taken into account. The standard

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approach to the continuum description of twin (or phase) boundaries is to use a multi-well energy landscape. Each minimum on the strain energy density represents an individual equilibrium phase or variant. It is necessary, however, to assume that the energy landscape is piecewise quadratic with a discontinuity in second derivatives (Abeyaratne and Knowles, 2006), or to deal with higher-order polynomials for elastic energy (the Landau-energy landscape framework (Falk, 1980; Rasmussen et al., 2001; Gu et al., 2013; Zoubková et al., 2022, c.f.)). Phase boundary velocity cannot be predicted uniquely in either case.

With the help of internal variables, this study clarifies how to represent twin boundary propagation at both slow and rapid speeds in the continuum mechanics framework. To keep things simple, we concentrate on a uniaxial scenario with a scalar transverse displacement field $u(x)$.

2 Uniaxial motion

In uniaxial setting, all fields are presumably dependent on a single coordinate and time. Transverse and longitudinal motions are uncoupled. We ignore longitudinal motion and focus entirely on shear strains. Restricting by the transverse displacement

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

we represent the balance of linear momentum in the isothermal case (without body forces) as

$$\rho v_t = \sigma_x. \tag{2}$$

Here σ is the shear stress, $v = u_t$ is the transverse particle velocity, ρ is the constant matter density, and subscripts denote derivatives. The kinematic compatibility condition reads

$$\varepsilon_t = v_x, \tag{3}$$

where $\varepsilon = u_x$ is the shear strain.

2.1 Jump conditions

Assume that a certain location x_0 corresponds to a potentially moving boundary $\mathcal{S}$ separating the variants. Within the context of continuum description, the following jump relation is satisfied at this boundary (Abeyaratne and Knowles, 2006, e.g.):

$$V_N \, [[\rho v]] + [[\sigma]] = 0. \tag{4}$$

Here V_N is the velocity of the moving twin boundary, and $[[B]] = B^+ - B^-$, $B^\pm$ are uniform limits of a field B in approaching the boundary from its positive and negative sides, respectively.

The latter relation is a consequence of the balance of linear momentum (2). A more complicated relationship is valid for the driving force $f_{\mathcal{S}}$ acting on the boundary (Abeyaratne and Knowles, 2006)

$$f_{\mathcal{S}} = [[W]] - \langle \sigma \rangle \, [[\varepsilon]] \,, \tag{5}$$

where W is the free energy per unit volume and $\langle ... \rangle$ denotes the arithmetical mean.

2.2 Velocity of the boundary

The velocity of the boundary is given by the relationship

$$\rho V_N^2 \, [[\varepsilon]] = [[\sigma]] \,, \tag{6}$$

which follows from jump relation (4) and that for the jump of the kinematic compatibility condition (3)

$$[[v]] = - \, [[\varepsilon]] \, V_N \,. \tag{7}$$

The direction of the boundary's velocity is determined by the entropy inequality on the boundary (Abeyaratne and Knowles, 2006)

$$f_{\mathcal{S}} V_N \geq 0. \tag{8}$$

It should be emphasized that the initial-boundary value problem lacks uniqueness because the stress jump in Eq. (6) is unknown in advance (Abeyaratne and Knowles, 1990). The difficulty can be overcome by introducing a new constitutive concept, namely, a kinetic relation, which relates the driving force with the velocity of the boundary (Abeyaratne and Knowles, 2006). However, things become even more complicated when twins are involved.

3 Isothermal twins equilibrium

We examine a material that could have two distinct twin variants. We consider both variants to be energetically equivalent, meaning that the energy value of the material points in both variants is the same in equilibrium. It is also assumed that the elastic parameters for both variants are the same. The elastic free energy per unit volume in a uniaxial condition is the quadratic function of shear strain

$$W = \frac{G}{2} \varepsilon^2. \tag{9}$$

Here G is the shear modulus of the material and subscript denotes the space derivative. It is evident that for both $+\varepsilon$ and $-\varepsilon$, the energy value is the same.

Assume that the variants occupy adjacent parts of a body separated by a twin boundary. We will look into the conditions needed for the variants to coexist in an equilibrium state. While there is no motion implied by the equilibrium state ($u = 0$), shear strains can be non-zero in both variants. Positive strains are related with variant 1, and negative strains with variant 2. It is commonly known that the strains in distinct twins differ from each other by the so-called transformation strain ε^{tr}. Due to the symmetry, the shear strain values can be given as follows::

$$\varepsilon_1 = \frac{1}{2}\varepsilon^{tr}, \quad \varepsilon_2 = -\frac{1}{2}\varepsilon^{tr}. \tag{10}$$

This ensures that the free energy remains equal in both variants. Here lower indices indicate twin variants. It is reasonable to suppose that in equilibrium, the stress value is zero. However, the stress is linear in strain

$$\sigma = \frac{\partial W}{\partial \varepsilon} = G\varepsilon, \tag{11}$$

which results in the following values of the stress in distinct variants:

$$\sigma_1 = G\varepsilon_1 = \frac{G}{2}\varepsilon^{tr}, \quad \sigma_2 = G\varepsilon_2 = -\frac{G}{2}\varepsilon^{tr}. \tag{12}$$

Consequently, stress equality cannot be realized in the equilibrium under macroscopic representation. Hence, twin equilibria and twin boundary motion become problematic for the macroscopic exposition. It is evident that the continuum description of twin boundary dynamics must be extended.

3.1 Internal variables

The idea of working with internal variables is not new. It has been used extensively in the modeling of shape memory alloys (Tanaka and Nagaki, 1982; Tanaka et al., 1986; Brinson and Huang, 1996; Auricchio and Lubliner, 1997). However, individual phase boundaries were generally avoided because the internal variable was the martensitic volume fraction with a specified transformation kinetics (Sadjadpour and Bhattacharya, 2007; Mirzaeifar et al., 2011; Song, 2020). Different versions of transformation kinetics have been reviewed in (Paiva and Savi, 2006; Khandelwal and Buravalla, 2009).

Another internal variable methodology is used in this work (Berezovski and Ván, 2017; Berezovski, 2018, 2023). Here, the distinction between the twins is characterized by internal variables. They can be used to estimate the velocities of twin boundaries.

We begin with a single internal variable case.

4 Single internal variable

In the single internal variable case, the free energy W per unit volume is specified as a quadratic function of the shear strain and the internal variable, γ (Maugin and Muschik, 1994, e.g.)

$$W = \frac{G}{2}\varepsilon^2 + \frac{1}{2}A\varepsilon\gamma + \frac{1}{2}C\gamma^2, \tag{13}$$

with material parameters $A = G\varepsilon^{tr}$ and C.

We assume that internal variable in twin variants has alternate signs in order to distinguish them. If variant 1 has the negative sign for the internal variable, then in variant 2 it should be positive. The shear stress is, by definition, determined as

$$\sigma = \frac{\partial W}{\partial \varepsilon} = G\left(\varepsilon + \frac{1}{2}\varepsilon^{tr}\gamma\right). \tag{14}$$

If $\gamma = -1$ then the value of the shear stress

$$\sigma_1 = G\left(\varepsilon_1 - \frac{1}{2}\varepsilon^{tr}\right), \tag{15}$$

corresponds to variant 1. For variant 2 we have, accordingly, $\gamma = 1$ and

$$\sigma_2 = G\left(\varepsilon_2 + \frac{1}{2}\varepsilon^{tr}\right). \tag{16}$$

4.1 Equilibrium conditions

Each twin variant's state is determined by the values of shear strains ε_1 and ε_2, as well as internal variable values γ_1 and γ_2, It is reasonable to suppose that both twins are stress-free in equilibrium. The following shear strain values correspond to zero stress levels:

$$\varepsilon_1 = \frac{1}{2}\varepsilon^{tr}, \quad \varepsilon_2 = -\frac{1}{2}\varepsilon^{tr}. \tag{17}$$

The driving force acting at the twin boundary reduces to the jump of the free energy in the stress-free equilibrium

$$f_S = [[W]] - \langle\sigma\rangle\,[[\varepsilon]] = [[W]]\,. \tag{18}$$

Calculating the free energy jump

$$
\begin{aligned}
(W_2 - W_1) &= \left(\frac{G}{2}\varepsilon_2^2 + \frac{1}{2}A\varepsilon_2\gamma_2 + \frac{1}{2}C\gamma_2^2\right) - \\
&- \left(\frac{G}{2}\varepsilon_1^2 + \frac{1}{2}A\varepsilon_1\gamma_1 + \frac{1}{2}C\gamma_1^2\right) = \\
&= \frac{G}{2}\left(\varepsilon_2^2 - \varepsilon_1^2\right) + \frac{1}{2}G\varepsilon^{tr}\left(\varepsilon_2\gamma_2 - \varepsilon_1\gamma_1\right) + \frac{1}{2}C\left(\gamma_2^2 - \gamma_1^2\right) + \sigma_0\varepsilon^{tr} = \\
&= \frac{G}{2}(\varepsilon_2 - \varepsilon_1)(\varepsilon_2 + \varepsilon_1) + \frac{1}{2}G\varepsilon^{tr}\left(\varepsilon_2\gamma_2 - \varepsilon_1\gamma_1\right) + \\
&+ \frac{C}{2}(\gamma_2 - \gamma_1)(\gamma_2 + \gamma_1) = 0,
\end{aligned}
\tag{19}
$$

we obtain zero value due to conditions $\varepsilon_1 + \varepsilon_2 = 0$ and $\gamma_2 + \gamma_1 = 0$. Therefore, there is no driving force at the twin boundary in equilibrium, as expected. The introduction of the internal variable allows the twins to achieve a stress-free equilibrium.

5 Slow motion

In order to ascertain the possible motion of the twin boundary, we must compute the driving force in a non-equilibrium situation

$$
\begin{aligned}
f_S = [[W]] - \langle\sigma\rangle\,[[\varepsilon]] &= \left(\frac{G}{2}\varepsilon_2^2 + \frac{1}{2}A\varepsilon_2\gamma_2 + \frac{1}{2}C\gamma_2^2\right) - \\
&- \left(\frac{G}{2}\varepsilon_1^2 + \frac{1}{2}A\varepsilon_1\gamma_1 - \frac{1}{2}C\gamma_1^2\right) - \frac{1}{2}(\sigma_2 + \sigma_1)(\varepsilon_2 - \varepsilon_1) = \\
&= \frac{G}{2}\left(\varepsilon_2^2 - \varepsilon_1^2\right) + \frac{1}{2}G\varepsilon^{tr}\left(\varepsilon_2\gamma_2 - \varepsilon_1\gamma_1\right) + \frac{1}{2}C\left(\gamma_2^2 - \gamma_1^2\right) + \\
&+ \frac{1}{2}\left(G(\varepsilon_2 + \frac{1}{2}\varepsilon^{tr}\gamma_2) + G(\varepsilon_1 + \frac{1}{2}\varepsilon^{tr}\gamma_1)\right)(\varepsilon_2 - \varepsilon_1) = \\
&= \frac{1}{2}G\varepsilon^{tr}\left(\varepsilon_2\gamma_2 - \varepsilon_1\gamma_1\right) + \frac{1}{2}C\left(\gamma_2^2 - \gamma_1^2\right) + \frac{1}{2}G\varepsilon^{tr}\langle\gamma\rangle(\varepsilon_2 - \varepsilon_1),
\end{aligned}
\tag{20}
$$

which is no longer zero. The twin boundary velocity is then computed as

$$
V_N^2 = \frac{[[\sigma]]}{\rho\,[[\varepsilon]]} = \frac{G(\varepsilon_2 + \frac{1}{2}\varepsilon^{tr}\gamma_2) - G(\varepsilon_1 + \frac{1}{2}\varepsilon^{tr}\gamma_1)}{\rho\,[[\varepsilon]]} = \frac{G}{\rho}\left(1 + \frac{\varepsilon^{tr}}{[[\varepsilon]]}\frac{[[\gamma]]}{2}\right). \tag{21}
$$

5.1 Asymptotics of the strain jump

For a small deviation of the actual shear strain jump from the value of the transformation strain, the shear strain jump can be represented in the form of an asymptotic expansion

$$[[\varepsilon]] = \varepsilon^{tr}(1 + \delta\epsilon^1 + \ldots), \tag{22}$$

with a small parameter δ. In the first approximation, the twin boundary's velocity in this case is

$$V_N^2 = \frac{G}{\rho}\left(1 + \frac{\varepsilon^{tr}}{[[\varepsilon]]}\frac{[[\gamma]]}{2}\right) \approx \frac{G}{\rho}\delta\epsilon^1, \tag{23}$$

because the value of $[[\gamma]]$ is close to 2 in the vicinity of twin boundary. It is evident that in a particular situation, the twin boundary velocity can be as small as that dictated by the value of δ. The slow motion of the twin boundary, corresponding to the single internal variable model, correlates with the results of quasi-static experiments (Faran and Shilo, 2011, 2016; Mizrahi et al., 2020; Shilo et al., 2021). However, the single internal variable model is unsuitable for fast dynamics of twin boundaries since it uses a parabolic evolution equation for the internal variable (Berezovski, 2018, 2023).

6 Dual internal variables and fast dynamics

We extend the diffusional description by using the dual internal variable technique (Berezovski and Ván, 2017; Berezovski, 2018). The complete theory of dual internal variables is presented in (Berezovski and Ván, 2017). In a simplified form of the theory, the free energy density is determined by internal variables γ and ψ using a quadratic function

$$W = \frac{G}{2}\varepsilon^2 + \frac{1}{2}A\varepsilon\gamma - \frac{1}{2}C\gamma^2 - \frac{1}{2}D\psi^2, \tag{24}$$

where material parameters $A = G\varepsilon^{tr}$, C, and D are constant. Negative signs for coefficients C and D are applied in the correspondence to (Berezovski, 2016).

Shear stress values are calculated as before

$$\sigma = \frac{\partial W}{\partial \varepsilon} = G\left(\varepsilon + \frac{1}{2}\varepsilon^{tr}\gamma\right). \tag{25}$$

6.1 Driving force and twin boundary velocity

For dual internal variables, the driving force is expressed as

$$
\begin{aligned}
f_S &= [[W]] - \langle\sigma\rangle\,[[\varepsilon]] = \left(\frac{G}{2}\varepsilon_2^2 + \frac{1}{2}A\varepsilon_2\gamma_2 - \frac{1}{2}C\gamma_2^2 - \frac{1}{2}D\psi_2^2\right) - \\
&- \left(\frac{G}{2}\varepsilon_1^2 + \frac{1}{2}A\varepsilon_1\gamma_1 - \frac{1}{2}C\gamma_1^2 - \frac{1}{2}D\psi_1^2\right) - \frac{1}{2}(\sigma_2+\sigma_1)(\varepsilon_2-\varepsilon_1) = \\
&= \frac{G}{2}\left(\varepsilon_2^2 - \varepsilon_1^2\right) + \frac{1}{2}G\varepsilon^{tr}\,(\varepsilon_2\gamma_2 - \varepsilon_1\gamma_1) - \frac{1}{2}C\left(\gamma_2^2 - \gamma_1^2\right) - \\
&- \frac{1}{2}D\left(\psi_2^2 - \psi_1^2\right) - \frac{1}{2}\left(G(\varepsilon_2 + \frac{1}{2}\varepsilon^{tr}\gamma_2) + G(\varepsilon_1 + \frac{1}{2}\varepsilon^{tr}\gamma_1)\right)(\varepsilon_2-\varepsilon_1) = \\
&= \frac{1}{2}G\varepsilon^{tr}\,(\varepsilon_2\gamma_2 - \varepsilon_1\gamma_1) - C\,[[\gamma]]\,\langle\gamma\rangle - D\,[[\psi]]\,\langle\psi\rangle - \frac{1}{2}G\varepsilon^{tr}\langle\gamma\rangle\,[[\varepsilon]]\,.
\end{aligned}
$$

The value of the twin boundary velocity is determined accordingly

$$
V_N^2 = \frac{[[\sigma]]}{\rho\,[[\varepsilon]]} = \frac{G(\varepsilon_2 + \frac{1}{2}\varepsilon^{tr}\gamma_2) - G(\varepsilon_1 + \frac{1}{2}\varepsilon^{tr}\gamma_1)}{\rho\,[[\varepsilon]]} = \frac{G}{\rho}\left(1 + \frac{\varepsilon^{tr}\,[[\gamma]]}{2\,[[\varepsilon]]}\right). \tag{26}
$$

6.2 Governing equations

The main distinction between single and dual internal variables approaches is that the evolution equation for the internal variable γ in the dual internal variable theory is hyperbolic (Berezovski, 2018, 2023)

$$
\frac{1}{D}\gamma_{tt} = C\gamma_{xx} - \frac{1}{2}A\varepsilon_x. \tag{27}
$$

It is convenient to introduce the time rate of the internal variable γ

$$
\gamma_t = w, \tag{28}
$$

In terms of the time rate, w, and the internal variable γ, we have the system of first-order equations

$$
Iw_t = C\gamma_x - \frac{1}{2}A\varepsilon_x, \tag{29}
$$

$$
\gamma_t = w_x, \tag{30}
$$

with $I = 1/D$.

Jump relations corresponding to Eqs. (29) – (29)

$$
V_N\,[[Iw]] + [[C\gamma]] = \frac{1}{2}A\,[[\varepsilon]]\,, \tag{31}
$$

$$
V_N\,[[\gamma]] + [[w]] = 0, \tag{32}
$$

can be combined to obtain the expression for the twin boundary velocity

$$V_N^2 \; [[I\gamma]] = [[C\gamma]] - \frac{1}{2} A \; [[\varepsilon]] \; . \tag{33}$$

Rearranging the latter relationship

$$(IV_N^2 - C) \; [[\gamma]] = -\frac{1}{2} A \; [[\varepsilon]] \; , \tag{34}$$

we can express the ratio between jumps of internal variable and shear strain

$$\frac{[[\gamma]]}{[[\varepsilon]]} = -\frac{1}{2} \frac{A}{(IV_N^2 - C)}. \tag{35}$$

Remembering the expression for the twin boundary velocity (Eq. 26)

$$V_N^2 = \frac{G}{\rho} \left(1 + \frac{\varepsilon^{tr} \; [[\gamma]]}{2 \; [[\varepsilon]]} \right). \tag{36}$$

we can eliminate jumps to obtain the relation

$$\frac{\rho}{G} V_N^2 - 1 = -\frac{\varepsilon^{tr}}{4} \frac{A}{(IV_N^2 - C)}, \tag{37}$$

which leads to the quadratic equation for the square of the twin boundary velocity

$$V_N^4 - \left(\frac{C}{I} + \frac{G}{\rho} \right) V_N^2 + \frac{G}{I\rho} \left(C + \frac{A\varepsilon^{tr}}{4} \right) = 0. \tag{38}$$

The solution of the quadratic equation

$$V_N^2 = \frac{1}{2} \left(\frac{C}{I} + \frac{G}{\rho} \right) \pm \sqrt{\frac{1}{4} \left(\frac{C}{I} - \frac{G}{\rho} \right)^2 - \frac{G}{I\rho} \frac{A\varepsilon^{tr}}{4}}. \tag{39}$$

depends only on material parameters.

If the transformation strain is sufficiently small then the velocity of the twin boundary is close to the shear wave speed in the material. This type of twin boundary dynamics is correlated with the propagation of twin tips (Takeuchi, 1966; Williams and Reid, 1971; Kannan et al., 2018).

7 Conclusions

Twin boundary motion and equilibrium of twins are not well described by classical continuum mechanics. The internal variable models utilized in the paper give further insight on the motion of twin boundaries. The simplest possible scenario (uniaxial motion with only two twin variants) was chosen to explain the experimentally observed discrepancies in twin boundary velocities. By incorporating internal variables into the continuum description of twin boundary motion, twin slow and fast dynamics can be theoretically distinguished. The velocity of a slow diffusional motion of a twin boundary is reproduced in the case of a single internal variable. In contrast, the dual internal variable approach provides fast dynamics of a twin boundary.

Acknowledgments

This research was supported by the Estonian Research Council under Research Project RPG1227.

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