

## Linear instability signals the initiation of motion of a twin plane under load

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This letter presents a study of the atomic mechanism of the initiation of motion of a static twin plane under applied mechanical load in a model shape-memory material. By tracking the deformation under load and using linear stability analysis, we find that the eigenvalues of the Hessian matrix provide an indicator of the initiation of motion of the twin plane. The initiation of motion is signaled by a linear instability and a drop in the lowest eigenvalue to zero as well as a sharp drop in higher eigenvalues. Additionally, by comparing with direct molecular dynamics, we see that the eigenmode associated with the zero eigenvalue is found to accurately predict the initial mode of motion. We also find that the initial motion occurs through the formation of a stacking fault just ahead of the existing twin plane and the broadening of the stacking fault drives further transformation.

**Keywords:** twinning; linear stability; kinetics of twin planes; molecular dynamics; shape-memory alloys

### 1. Introduction

Crystallographic twin boundaries are microstructural interfaces with different crystal structures on either side. The crystal structures on either side are symmetry-related as well as related by a shear deformation. An important feature of twin interfaces is their coherence with the registry of atoms on either side. This enables twin boundaries to play a key role in a number of important engineering materials, such as functional alloys and nanotwinned materials. In functional materials such as shape-memory alloys [1] and ferromagnetic shape-memory materials [2], the coherence of the twin boundaries is a factor in allowing atoms to maintain neighbors despite apparently plastic deformations, thus enabling shape memory. Our motivation is to understand the dynamic response of shape-memory alloys that is governed by the nucleation and motion of the twin boundaries.

Many efforts in this area have concentrated on constructing continuum models of twin boundary motion [3]. Predictive continuum models of this phenomenon require

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atomistic understanding. Recent atomistic studies of the twin-boundary motion include, e.g. the analysis of steady motion in model one-dimensional systems [4,5], more realistic studies of the twin-boundary motion in higher dimensions [6–8], and studies of the twin boundary nucleation in atomic-like continuum theories [9]. An important aspect of the motion of twin planes that has received relatively little attention is the mechanism of initiation of motion when subjected to mechanical load. In this letter, we present an atomic-level study of this process. We use a model two-dimensional 2D atomic system that is based on the shape-memory Ni–Mn alloy. Our calculations demonstrate that the initiation of motion of a twin boundary is signaled by a loss of linear stability, i.e. the Hessian matrix has a zero eigenvalue or *soft mode* immediately prior to initiation of motion. Additionally, a number of higher modes are coupled to the soft mode and there is a corresponding drop in those eigenvalues as well. By comparison with direct molecular dynamics calculations, we further find that the soft eigenmode associated with the zero eigenvalue is an accurate indicator of the initial mode of propagation of the twin boundary. Finally, our calculations and analysis show that the initial motion of a twin boundary occurs through the formation of a stacking fault immediately in front of the existing twin plane, and its subsequent merger with the existing twin.

## 2. Method

Our work uses some of the formulation from the 2D study of model shape-memory Ni–Mn by Hildebrand and Abeyaratne [6]. They have examined the motion of twin boundaries under far-field shear stress, using a biatomic Lennard–Jones (LJ) system that is fit to reproduce the lattice parameters and square-to-rectangle phase transformations. We use their atomic potentials because they are well-characterized and provide the necessary crystallographic symmetries that we desire. The interaction between the atoms  $i$  and  $j$  atoms is

$$\Phi_{\alpha\beta}(r_{ij}) = 4\epsilon_{\alpha\beta} \left( \left( \frac{\sigma_{\alpha\beta}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{\alpha\beta}}{r_{ij}} \right)^6 \right), \quad (1)$$

where  $\epsilon_{\alpha\beta}$  and  $\sigma_{\alpha\beta}$  are the energy scale and length scale parameters, respectively, in the LJ interaction potential between species  $\alpha$  and  $\beta$ , with  $\alpha$  and  $\beta$  corresponding to either Ni or Mn. The values of these parameters are listed in Table 1 after having been nondimensionalized by setting  $\sigma_{NiNi}$  and  $\epsilon_{NiNi}$  as unit length and energy. The quantity  $r_{ij}$  denotes the distance between atoms  $i$  and  $j$ .

Table 1. Nondimensional LJ parameters in 2D Ni–Mn system.

$\alpha - \beta$	Ni–Ni	Ni–Mn	Mn–Mn
$\sigma_{\alpha\beta}$	1.0	1.0205	0.8736
$\epsilon_{\alpha\beta}$	1.0	0.9810	0.9905

We use a shifted LJ potential to enable a smooth cutoff at  $4.5\sigma_{NiNi}$ . The lattice parameters of this potential are listed in Table 2. The potential energy of a system of atoms with positions  $\{\mathbf{r}\}$  at equilibrium is given by

$$E(\{\mathbf{r}\}) = \sum_i \sum_j \Phi_{\alpha\beta}(r_{ij}) - \underbrace{\sum_i \mathbf{F}_i \cdot \mathbf{r}_i}_{\text{boundary work}}, \quad (2)$$

with  $\mathbf{F}_i$  being the external force applied to the boundary atom labeled by  $i$ , and the Hessian is  $\frac{\partial^2 E}{\partial r_i \partial r_j}$ .

Our calculations are set up as follows. Figure 1 shows a schematic of the initial configuration of the atoms. The system is periodic with 40 atoms in the horizontal direction and finite in the vertical direction with 120 rows of atoms. The top 40 rows and the bottom 40 rows are initialized to be in Variant 1, and the remainder in the middle are in Variant 2, giving rise to two twin planes. The lattice is aligned such that the twin planes are horizontal. In a previous study with a single twin plane, nucleation of new twins at the boundary of the simulation domain was observed

Table 2. Lattice parameters in 2D Ni–Mn system.

Phase	Square	Rectangle (Variant-1)	Rectangle (Variant-2)
Length	1.33603	1.14101	1.54110
Width	1.33603	1.54110	1.14101

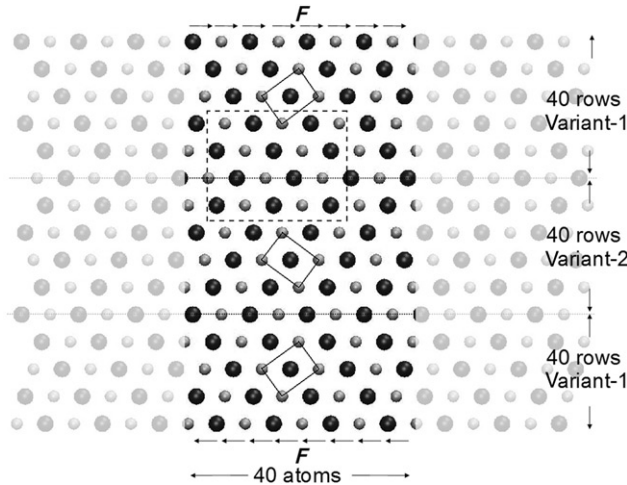


Figure 1. The simulation cell contains 4800 atoms: 20 Ni and 20 Mn atoms in each of the 120 rows. Periodic boundary conditions are applied in the horizontal direction, and forces are applied parallel to the twin boundaries on the outermost atoms. Variant 1 and Variant 2 are defined through the sketch above. The box surrounded by the dashed lines is shown in greater detail in Figure 2.

rather than twin plane motion [6]. Hence, we use two symmetrically placed twin planes to suppress boundary nucleation and enable us to focus on twin plane motion.

We begin with a lattice that is not loaded by boundary forces and is also relaxed with respect to the periodicity in the horizontal direction. We then apply forces  $F$  to the outermost rows of atoms at the top and at the bottom in the direction shown in Figure 1 to mimic a shear stress. Starting from  $F=0$ , we increase  $F$  in positive increments  $\Delta F$ . Under this load, Variant 1 is energetically preferred to Variant 2, but there is an energetic barrier to transformation. Hence, a finite load is required for the twin planes to begin moving towards each other. After applying a load increment  $\Delta F$ , we use a conjugate gradient algorithm to equilibrate with the final atomic configuration from the previous load step as the initial guess. In addition to relaxing the atomic positions, we also relax with respect to the periodic spacing in the horizontal direction to relieve possible stresses in that direction. At each equilibrium configuration, we calculate the lowest 10 eigenvalues of the matrix of second derivatives of the energy with respect to the atomic positions (i.e. the Hessian). Hence we are able to track the evolution of the eigenvalues as the system is loaded. If the load step causes motion or other rearrangement that cannot be reversed by releasing the load, we reduce the value of the load increment and repeat the calculation from the previous load level. This bisection approach gives us an accuracy of  $10^{-6}$  in nondimensionalized units in calculating the critical load and the configuration immediately prior to the twin boundary motion and eliminates unwanted dynamical effects.

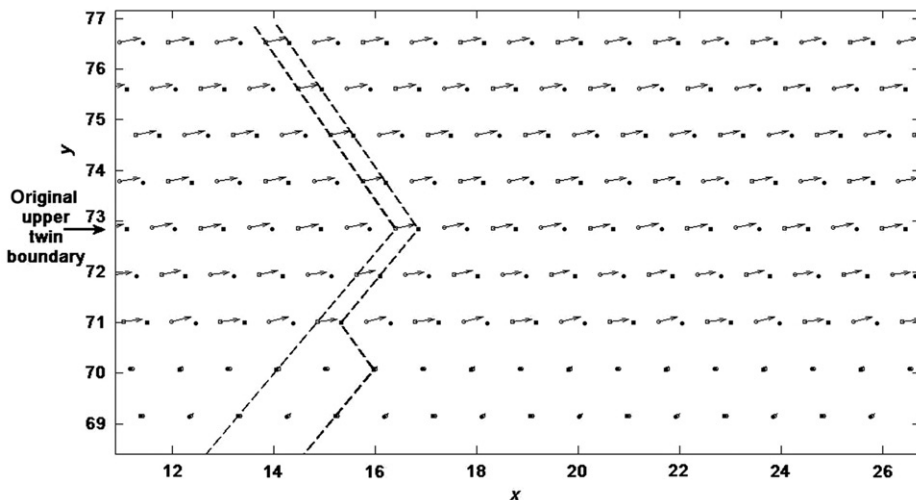


Figure 2. Atomic displacements at the twin boundary. Open circles and squares show the positions of Ni and Mn just before rearrangement, and filled circles and squares show the positions just after rearrangement. The dashed lines are to aid understanding. The arrows display the soft eigenmode matching the observed displacements.

### 3. Results

Figure 2 shows the atomic configuration just before the twin planes begin motion as well as the equilibrium configuration just after that. The top portion of the crystal above the twin plane undergoes an almost rigid translation. However, two rows of atoms below the twin plane also translate to the right in a coordinated manner. Beneath these two rows, there is almost no displacement. This entire coordinated motion occurs within *a single iterate* of the conjugate gradient at the critical load. The net result of this displacement is the formation of a stacking fault that can also be considered as a pair of newly nucleated twin planes that are immediately adjacent to each other. Upon further loading, these twins move apart and cause further transformation to the energetically preferred variant.

Throughout the loading process, we track the 10 lowest eigenvalues of the Hessian matrix, plotted in Figure 3. All eigenvalues are positive and do not change much until we approach the critical load (whose normalized value is  $\sim 1.05$ ). At that point, the lowest eigenvalue goes to zero and the higher eigenvalues also drop sharply

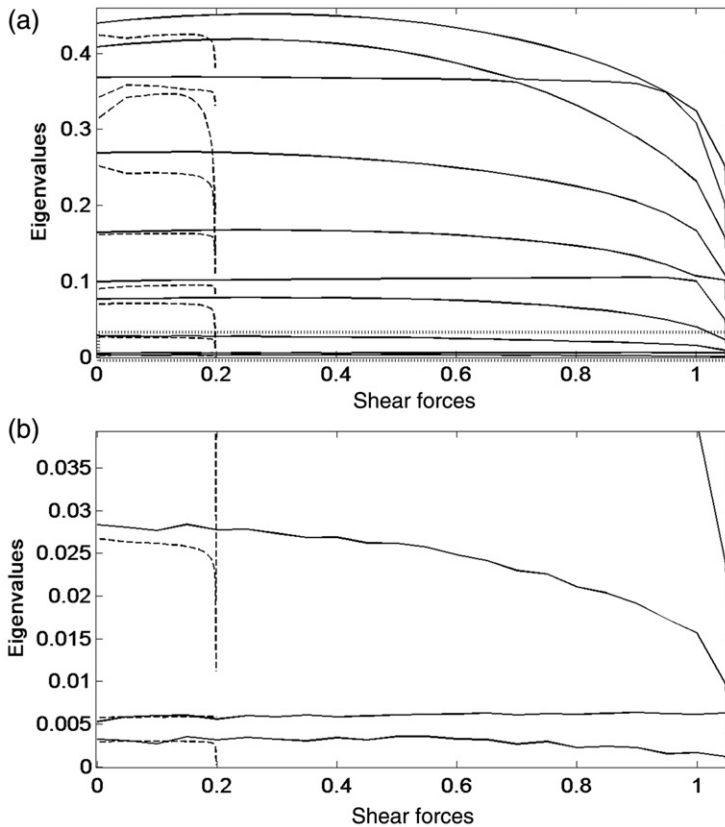


Figure 3. The lowest 10 eigenvalues plotted against force. (a) Solid lines are with ideal twin boundaries; dashed lines are with weakened twin boundaries. (b) The lower part of (a), shown by the dashed lines, is enlarged to show the lowest three eigenvalues.

though they remain positive. We plot the soft eigenmode associated with the zero eigenvalue in Figure 2. We see that it matches well with the observed atomic displacements. In the lower part of the figure, the displacements are very small and hence the arrows are not visible. We further test the soft-mode prediction against direct damped molecular dynamics. The use of this alternate method enables us to rule out the possibility that our findings are numerical artifacts generated by a particular choice of evolution algorithm. Figure 4 presents snapshots of the molecular dynamics calculation. We observe the system at a number of different times, and the atomic motion shows the formation of a stacking fault in agreement with soft eigenmode predictions.

To confirm that our findings are not due to other instabilities such as plastic slip causing softening of the eigenvalues, we perform similar calculations with an interface that is weakened by substituting Ni for Mn on a few sites located on the twin plane. We observe from Figure 3 that the critical load is reduced by a factor of about 5. However, our conclusions continue to hold. In particular, the lowest eigenvalue again goes to 0 at the corresponding critical load and the other eigenvalues sharply drop off, and the soft mode again predicts the coordinated motion of the atoms and stacking fault formation that agrees with corresponding molecular dynamics simulations. We have also tested the robustness of our conclusions with larger system sizes, with the largest being, in comparison to that described in the paper, 16 times as large in the horizontal direction and 8 as large in the vertical direction. We also note that if we do not relax the periodicity in the horizontal direction but instead keep it fixed, the critical load is slightly increased but there are no qualitative or significant quantitative changes in our results.

#### 4. Discussion

In conclusion, we find that the initiation of motion of the twin boundary interface subjected to far-field loads can be predicted by examining the spectrum of the Hessian matrix. The lowest eigenvalue going to 0 signals the initiation of motion, and the corresponding eigenmode predicts the initial mode of motion of the twin boundary as a coordinated movement of atoms that forms a stacking fault ahead of the twin plane. Our findings show some contrasts to the higher temperature calculations of Hildebrand and Abeyaratne [6]. In particular, they observe that rather than existing twins moving under applied loads, there are new twins nucleated at the boundaries of the computational domain. They also find when these newly nucleated twins move by the motion of kinks that traverse the width of the interface, rather than the interface moving as a single front as we observe. It is likely that these differences reflect the role of kinetic energy, as well as the fact that twin boundaries in their calculations involve the nucleation and initiation of the twin boundary motion in a manner that does not allow a direct distinction between the two processes. It is possible that the mode of motion (kinks or front) is sensitive to the initial stages of transition from static to moving.

We also mention recent efforts to explore the energetic landscape of other shape-memory alloys using accurate DFT calculations [10]. In this work and related papers by the same authors, the deformation mode is assumed to be front motion

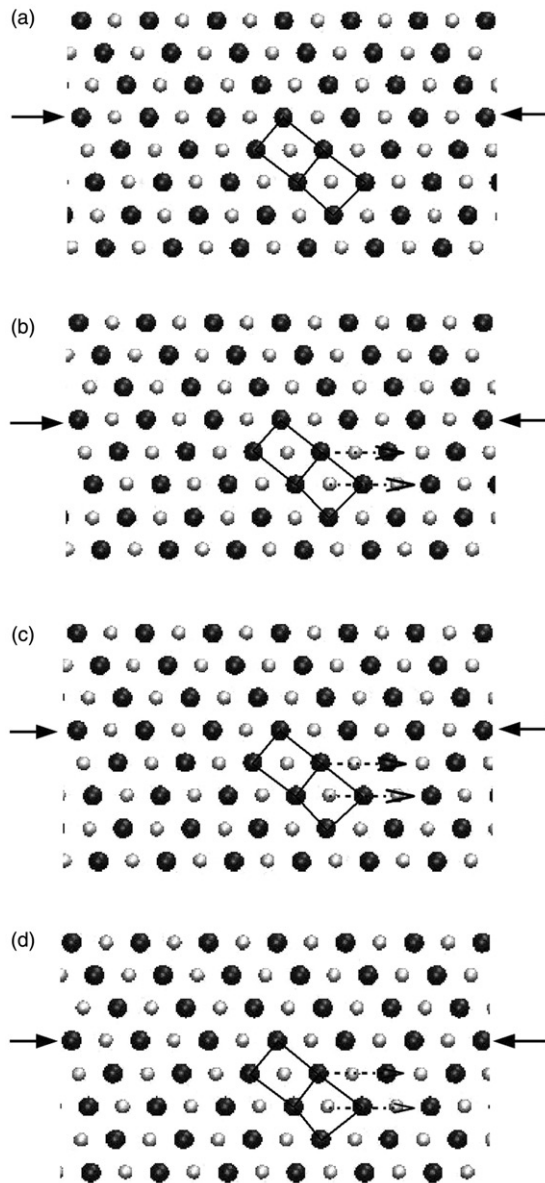


Figure 4. Snapshots for the region near the upper twin boundary in the MD simulation. Solid arrows indicate the original twin boundary, and dashed arrows indicate the direction in which the atoms move. (a)  $t=152,000$ , just before the motion is initiated. (b)  $t=161,000$ . (c)  $t=167,000$ . (d)  $t=171,000$ . The time step is 0.001.

rather than kink motion. DFT calculations along the assumed path are then used to estimate critical twinning stress and other quantities of interest. The critical stress is found to agree well with experiments, suggesting the possibility that the deformation mode that they assume and we predict is indeed a mechanism of twin motion.

We note that linear stability analyses have successfully predicted the nucleation of microstructural defects, e.g. dislocations [11], phase boundaries [9], and cracks [12]. However, the connection between the initiation of motion of the twin boundaries and the linear instability has not been previously demonstrated. This link can allow us to study this phenomenon using bifurcation approaches [13]. This connection may also provide ways to understand structural nanotwinned metals that show very promising properties [14–17].

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