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Structural origin of reversible martensitic transformation and reversible twinning in NiTi shape memory alloy

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ABSTRACT

Much progress has been made over the past few decades in resolving the mechanism for the transformation from ordered body-centered-cubic (B2) austenite to monoclinic martensite (B19') in NiTi shape memory alloy, as well as the twinning mechanisms in martensite. However, so far no lattice correspondence analyses on the atomic scale have been conducted, as a result, these mechanisms have not been completely understood in terms of the pathways for reversible phase transition and reversible twinning in martensite. In this work, atomistic simulations were performed to investigate how B2 austenite transforms to B19' martensite and how twins are formed during phase transformation. In particular, lattice correspondence in the structural evolutions was carefully analyzed to reveal the martensitic transformation mechanism and twinning mechanism with much better clarity. The simulation results show that, when martensite grains were nucleated in austenite, they already formed a twin relationship as a natural result of the crystal structure. Thus, self-accommodation is achieved naturally. Coalescence occurred subsequently and some martensite grains grew at the expense of their neighbors, indicating that the interfaces are elastically mobile and their migration is reversible. Eventually twinned martensite variants were created. It is shown that, in the B2 $\rightarrow$ B19' transformation, the B19' monoclinic structure can be treated as a distorted hexagonal close-packed (HCP) structure. With this treatment, it is demonstrated that the martensitic transformation is essentially similar to BCC $\leftrightarrow$ HCP transformation which only involves atomic shuffles and is reversible, and twinning in martensite is essentially similar to $\{10\bar{1}2\}$ twinning in HCP metals which only involves atomic shuffles and is reversible as well. Another significant discovery is that the B19' martensite exhibits a very special dual-lattice structure: the relatively weak Ti-Ti bonding of the monoclinic unit cell permits easy reorientation of lattice units. As a result, two differently oriented lattice units co-exist in the same martensite grain which loses long range periodicity, providing an extra degree of freedom for accommodating external and internal strains. These results explain well why B19' martensite is extremely adaptive to straining and why deformation is reversible.

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1. Introduction

Equiatomic NiTi alloy is a member of a class of functional materials that present shape memory effect (SME) [1]. At room temperature (RT), the stable phase of NiTi is martensite with a B19' monoclinic crystal structure. The martensite phase can be deformed plastically at RT, but upon heating, the martensite transforms to austenite which has a B2 ordered structure, and the material recovers its original shape before deformation. SME has been applied to numerous engineering applications [2–4] and the underlying physics that accounts for SME is of particular interest to researchers.

In addition to thermal SME including one-way or two-way [5,6], mechanical SME (pseudoelastic) [7,8] and twinning induced SME were also observed in shape memory alloys [9]. It has been established that SME in NiTi originates from two physical processes [9–12]. The first one is B2 $\leftrightarrow$ B19' reversible martensitic transformation and the second one is twinning in martensite, which should presumably be reversible as well for whatever driving mechanisms. Dislocation activities should make no or negligible contribution during deformation because dislocation slip is generally chaotic and irreversible once dislocations glide out to free surfaces, pile up or entangle near interphase boundaries and grain boundaries or interact with other crystalline defects. Conceivably, migration of martensite-austenite interphase boundaries and twin boundaries in martensite should be free of dislocations as well in order for a metal to have SME. Over the past few decades, extensive research

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has been conducted to resolve the mechanisms for martensitic transformation and twinning in NiTi alloy [5,13–18].

The crystallography of $B2 \rightarrow B19'$ martensitic transformation was investigated in the pioneering work by Knowles and Smith [19]. They conducted transmission electron microscopy (TEM) experiments on the twinned martensite and applied phenomenological theory [20] to predict possible twinning modes in martensite. Type II $\eta_1 = [011]$ mode, type I $K_1 = (11\bar{1})$ mode and type I $K_1 = (001)$ mode were examined mathematically. These predictions were based on the assumption of lattice invariant shear that minimizes the overall shape strain. Extensive TEM observations of twins in martensite in NiTi were also conducted by Nishida et al. [21–23]. In addition to the twinning modes described by Knowles and Smith [19], Nishida et al. further categorized type I $K_1 = (11\bar{1})$ mode into three types – deformation twins, accommodational variants and lattice invariant twins. (100) and (001) compound twinning modes were considered deformation twins. Moreover, they reconfirmed type I $K_1 = (011)$ lattice invariant twins. It is worth noting that, due to the low symmetry of the B19' martensite, it is not easy to tilt a TEM thin foil and then definitively identify the zone axis of the twins. Another limitation comes from the limited range of tilt angle of a TEM sample stage. Thus, uncertainties arise and more TEM research is needed to substantiate such a multiplicity of twinning modes in the low symmetry B19' structure and to ascertain the nature of those reported twin variants.

In recent years, computer simulations have been used to study martensitic transformation and SME in metals. The simulation work by Shao et al. [10] is one of the earliest atomistic simulations of martensitic transformation in shape memory NiAl alloy. In their work, $B2 \rightarrow BCT$ martensite nucleation and growth were simulated by using embedded atom method (EAM) [24,25] potential for Ni–Al binary alloys [26]. They showed that, twin domains were formed immediately after the martensite was nucleated. Their results indicated that the interface between austenite and martensite, and the interface between twin variants remained elastic or dislocation-free so that the migration of these interfaces was reversible. Ishida and Hiwatari [27] developed a modified embedded atom method (MEAM) [28] potential and simulated martensitic transformation in NiTi. They reported that straining and atomic shuffles produced a $B2 \rightarrow B19$ orthorhombic structure. A subsequent simple shear along the $(110)[1\bar{1}0]_{B2}$, which corresponds to the $(100)[00\bar{1}]_{B19}$, transformed the B19 to the final B19' martensite, and the martensitic transformation was reversible. Ko et al. [29,30] developed a MEAM potential for Ni–Ti–V and used it to simulate phase transformation in nanocrystalline a NiTi alloy. Reversible $B2 \leftrightarrow B19'$ transformation was observed in thermally-activated or stress-induced conditions. Ren and Sehitoglu [31] developed a Finnis–Sinclair (FS) interatomic potential which is able to reproduce physical properties of B2, B19 and B19' phases, and the temperature dependent stability of martensite. These pioneering works provided little details on structural evolution, especially lattice transformation in phase transition and twinning. A considerable amount of work has been focused on the energetics calculations of possible twin variants in B19' martensite, which is a key feature in shape memory alloys. Using density functional theory (DFT) [32–34], Sehitoglu et al. [35–45] conducted extensive calculations of the energy landscape of possible twinning or slip planes. This method is based on the concept of generalized planar fault energy (GPFE) [46,47] which describes the energy barrier when an atomic plane shears against its neighboring plane along a certain crystallographic direction. Martensitic transformation in shape memory alloys has also been investigated by researchers using continuum mechanics based modeling [48–51].

Despite the research efforts over the past few decades, a fundamental issue regarding the origin of reversible martensitic transformation and reversible twinning in martensite is still not fully

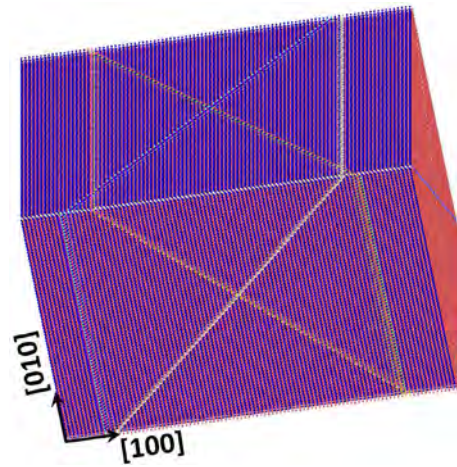


Fig. 1. The initial configuration of B2 austenite Ni50Ti50 shape memory alloy. The red atoms are Ni, and blue atoms Ti. Pairs of {110} planes are pre-selected and colored differently for the purpose of lattice correspondence analyses. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

understood. As suggested by Clapp [10], the reversibility of these two physical processes implies that the interphase boundaries and the intervariant boundaries have to be elastic or dislocation-free. On the atomic scale, how such a reversibility is achieved remains unclear. The purpose of this work is to resolve this fundamental issue, using lattice transformation analysis on the results obtained from atomistic simulations. Specifically, transformations of crystallographic planes of austenite to the corresponding planes of martensite are carefully tracked and analyzed.

2. Simulation method

Several interatomic potentials for Ni–Ti system have been developed by a number of researchers [29–31]. The atomistic simulations in this work were performed by using the most recently developed modified embedded atom method (MEAM) [28] interatomic potential for Ni–Ti by Ko et al. [52]. This potential describes well phase transformations in Ti and equiatomic NiTi. The initial configuration of a single crystal B2 austenite is shown in Fig. 1. In this plot, the Ni atoms are plotted in red and the Ti atoms in blue. The dimension of the single crystal austenite is $31 \times 22 \times 22$ nm, containing a total of about 1.0 million atoms. Free surfaces were applied to all three dimensions. The temperature of the system was maintained at 100 K. At this temperature, the B2 austenite is unstable and transforms to B19' martensite which has a monoclinic structure. The time step size was chosen as 1.0 fs.

A special feature in Fig. 1 is that pairs of {110} planes of the B2 structure were pre-selected and colored differently. The color patterns were retained throughout the simulations. Thus, during martensitic transformation and twinning, these pre-selected {110} planes would be transformed to their corresponding planes in martensite and twin. By tracking the transformations of these planes and others, the lattice correspondence between austenite and martensite, parent and twin can be established unambiguously. Such an analysis offers highly valuable insight with regard to the mechanisms of phase transformation and twinning.

3. Results

Shortly after the simulation started, martensite grains were quickly nucleated inside the austenite parent. We first show the cosmetic change of the system, as displayed in Fig. 2. It can be observed that distortion and surface relief took place in the initial B2

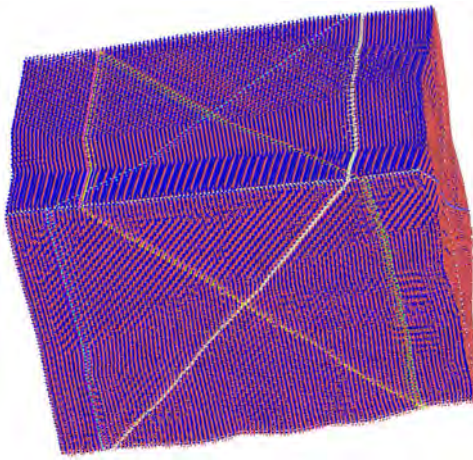


Fig. 2. The final configuration of the system after martensitic transformation. The B2 austenite has transformed to monoclinic B19' martensite. Surface relief can be observed after martensitic transformation.

structure, indicating that phase transformation occurred. The traces of the pre-selected $\{110\}$ planes are distorted or deflected, which is typical of martensitic transformation.

For the convenience of presenting the simulation results, analyses and discussion, it is necessary to define the coordinate systems for our simulations. The definition is shown in Fig. 3. First, a group of atoms are selected from the initial B2 austenite, as shown in Fig. 3a from which the BCC structure can be seen. The plot is very slightly tilted to show the BCC lattice in 3D. Then the configuration of this same group of atoms are plotted at a time step

when martensitic transformation is complete. The structure of the selected atoms in the martensite is shown in Fig. 3b. The viewing direction of Fig. 3b is nearly the same as that of Fig. 3a. This way, the structure of the B2 austenite and the B19' martensite can be directly compared and lattice transformation can be inferred definitively. Fig. 3b is actually the projection view of the B19' structure along the a -[100] direction. The axes of b -[010] and c -[001] are marked out in the plot. The b and c axes and the dashed green lines constitute the (100) face which is one of the three faces of the B19' unit lattice.

Next, we use the same group of atoms, but tilt them such that the viewing direction is exactly along the $[1\bar{1}0]$ direction of the initial B2 structure (Fig. 3c). The corresponding B19' structure after martensitic transformation is shown in Fig. 3d. This viewing direction is exactly along the c -[001] direction of the B19' unit lattice. The a and b axes of the B19' are marked out. The a , b , and c axes constitute the coordinate system of the martensite. The angle between the a and b axes is about 97° . The green lines in Fig. 3d constitute the (001) face of the monoclinic lattice.

From the plots in Fig. 3, it can be readily seen that, during $B2 \rightarrow B19'$ martensitic transformation, the (110) plane of austenite is transformed to the (001) plane of martensite, and the $(1\bar{1}0)$ plane of austenite is transformed to the (010) plane of martensite, and the (100) plane of austenite is transformed to the (100) plane of martensite. These transformations can be described as:

$$(001)_{B2} \rightarrow (100)_{B19'};$$

$$(110)_{B2} \rightarrow (001)_{B19'}; \text{ and}$$

$$(1\bar{1}0)_{B2} \rightarrow (010)_{B19'}.$$

The three lattice parameters of the monoclinic unit cell obtained from the simulation are: $a = 0.286$ nm, $b = 0.459$ nm,

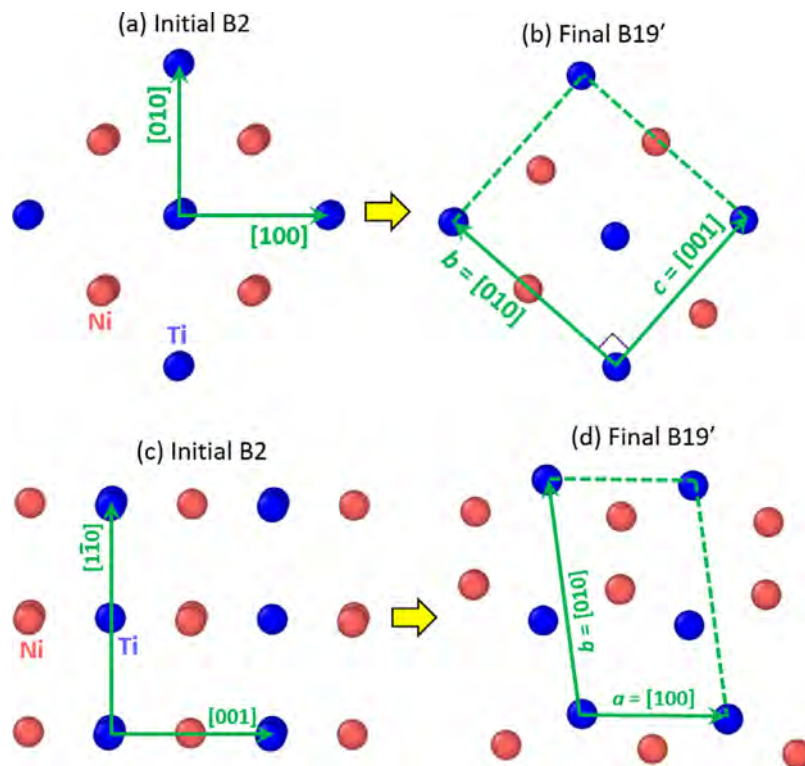


Fig. 3. The coordinate system for the B2 austenite and the B19' martensite. A group of atoms are selected from the simulation, and the initial and final configurations are plotted. The red atoms are Ni, and blue atoms Ti. (a) The initial B2 austenite when viewed along the [001]. (b) The final B19' martensite transformed from (a). The b and c axes of the monoclinic unit cell are labelled out. The viewing direction is along the a -axis of the monoclinic unit cell of which the (100) face is delineated by the green lines. (c) The initial B2 austenite when viewed along the $[110]$. (d) The final B19' martensite transformed from (c). The viewing direction is along the c -axis of the monoclinic unit cell of which the (001) face is delineated by the green lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

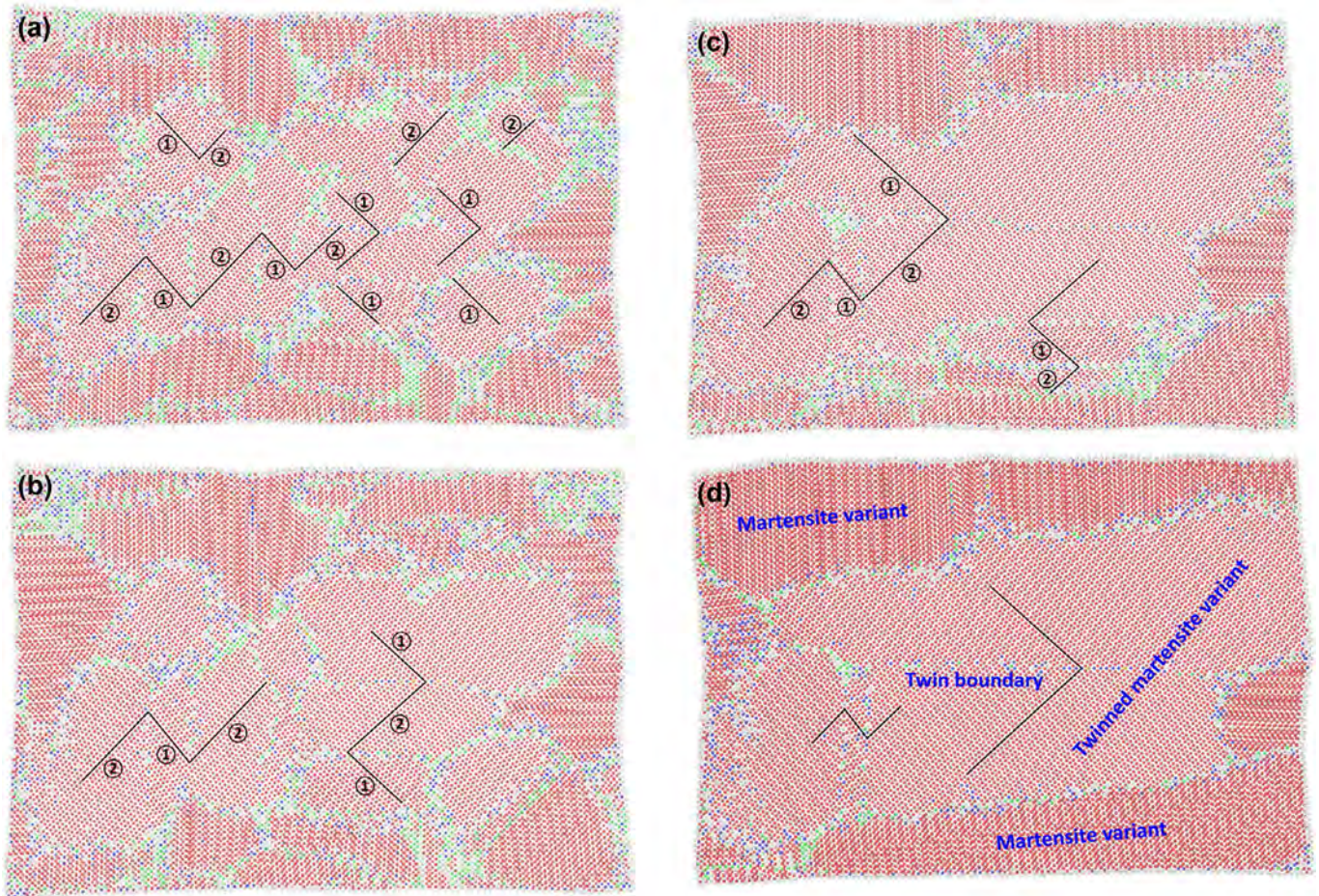


Fig. 4. Structural evolution in time sequence during martensitic transformation. Only a thin slice is shown. Bond angle analysis (BAA) [53] is used to distinguish different structures. The red atoms are B19' martensite. Atoms of other colors are located at grain boundaries and surfaces. (a) Early stage of martensitic transformation. Numerous martensite grains are formed. The black lines mark the traces of (001) planes. The marked-out grains have two orientations. (b) Coalescence of the martensite grains. Some grains are growing at the expense of their neighbors. (c) More coalescence is occurring while some grains disappear. (d) The final structure of martensite. The grains form twin relationship. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$c = 0.414$ nm, and the angle between axes a and b is $\sim 97^\circ$. These parameters agree well with experimental data.

With the coordinate system defined in Fig. 3, we can now show more details of structural evolution during martensitic transformation obtained in our simulations. The results are shown in Fig. 4. To generate the plots of atomic configurations, bond angle analysis (BAA) is used [53]. Common neighbor analysis (CNA) [53] works less well in revealing the crystal structure because of the low symmetry of the B19' monoclinic structure. Only a thin slice (0.5 nm thick) of the system is shown, and the snapshots are displayed in time sequence. As shown in Fig. 4a which corresponds to the early stage of martensitic transformation, atoms of the B19' monoclinic structure are shown in red, whereas atoms on the grain boundaries are shown in green and blue and atoms on the free surfaces mostly in white. It is clearly seen that multiple martensite grains had been nucleated shortly after the simulation started. The martensite grains are oriented differently, indicating that multiple variants are formed. The grains in the central region of the plot happen to be right in the zone axis which is the [100] and these grains show a well-defined monoclinic lattice structure of B19'. Black lines are drawn parallel to the trace of (001) planes. It can be seen that these martensite grains already form a twin relationship. By carefully tilting the thin slice, we found that other martensite variants off the zone axis near the free surfaces have exactly the same crystal structure as those grains in the central region.

As the simulation proceeds, very interestingly, the martensite grains coalesce and coarsen (Fig. 4b). Some grains are growing at the expense of their neighbors. Obviously, the interface between the martensite grains are highly mobile. Again, the traces of (001) planes of the martensite grains are denoted by the black lines and the twin relationship can readily be observed.

Coalescence between the martensite grains continues as the simulation time further increases (Fig. 4c). Eventually, two dominant martensite grains are formed in the central region. Still, a few smaller grains can be seen, but these grains, regardless of grain size, form a twin relationship, as indicated by the black lines. Eventually, some of the small grains disappear and are totally consumed by the large grains. For example, the two martensite twins near the bottom entirely disappear, as shown in Fig. 4d. In the central region, two large martensite grains are formed and they satisfy a well-defined twin relationship. At the top and bottom of the plot, large martensite grains are formed as well, but they are oriented differently and off the zone axis.

To better reveal the structure of the martensite grains, a magnified view of B19' twins is shown in Fig. 5 with bond angle analysis turned off. In this plot, the Ni atoms are shown in red and Ti atoms in blue, the same as in Fig. 1. A region near the twin boundary is magnified and plotted. The dashed lines denote the traces of (001) planes of the twins. The zone axis is along the [100]. The solid black lines denote the twin boundary. A step on the twin boundary can be seen. Note that the twin boundary exactly coincides with

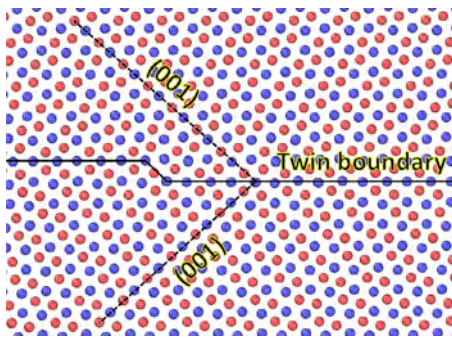


Fig. 5. A magnified view of B19' twins in Fig. 4d with bond angle analysis turned off. The red atoms are Ni, and blue atoms Ti. The color patterns of the pre-selected atomic planes are turned off. The solid black lines denote the twin boundary which is on the (011) plane. A step on the twin boundary can be seen. Note that the twin boundary exactly coincides with the Ti atomic plane (the blue atoms) and it cannot be on Ni or Ni-Ti atomic planes due to the monoclinic structure. The dashed lines denote the traces of (001) planes of the twins. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

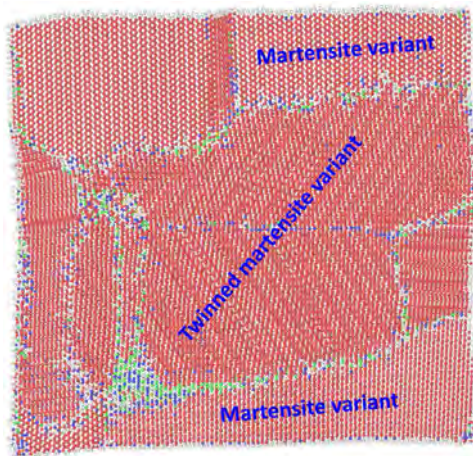


Fig. 6. When Fig. 4d is tilted around the vertical direction such that the viewing direction is right along the *c*-axis, i.e. [001] of the top martensite variant, the (001) plane of the variant can be well observed. In contrast, the twinned martensite in the middle is now off the zone axis of [100].

the Ti atomic plane and it cannot be on Ni or Ni-Ti atomic planes due to the monoclinic structure, irrespective of the orientation of the twins. After we carefully examined the structure of most of the twin boundaries, we found that this is always the case. An explanation is provided in the analysis section below.

Those martensite grains off the zone axis and near the free surfaces have the same B19' monoclinic crystal structure. This can be seen when those grains are tilted to a specific zone axis, as shown in Fig. 6. The martensite variant near the top surface in Fig. 4d is tilted such that the viewing direction is along the *c*-[001] direction, and the structure of (001) plane can be observed. Similar examinations reveal that other martensite variants have the same monoclinic structure as well.

Fig. 4 shows that there are two twinning planes for those martensite grains that are right on the zone axis. In addition to the nearly horizontal twinning plane (Fig. 5), the smaller grains have twin boundaries that are nearly vertical. This is better revealed in Fig. 7. In this plot, another slice is taken out at a different location. The twinned martensite can be clearly observed but the twin boundaries are nearly vertical. Inside the martensite grains, there are interfaces (indicated by the blue arrows); but on both sides of these interfaces, the martensite grains have the same orientation.

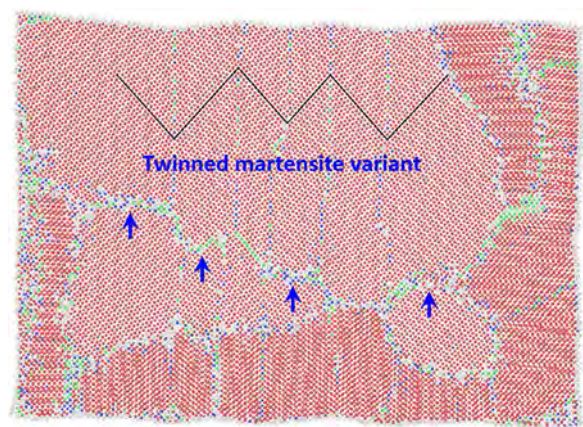


Fig. 7. Another set of twinned martensite. The viewing direction is the same as that in Fig. 4. The arrows denote the disregistry inside the martensite grains. The disregistry was created when two martensite grains with the same orientation met during growth and coalescence.

This disregistry inside the martensite grains are generated during coarsening and coalescence of martensite grains. When two grains with the same orientation meet during growth, if the two lattice are not exactly aligned in phase, such disregistry and stacking fault can be created.

4. Analysis and discussion

4.1. Lattice transformation in B2 → B19' martensitic transformation

Our simulation results (Figs. 4d and 7) reveal well-defined twin structure between B19' martensite grains produced in thermally induced phase transition in NiTi. These twins are initially nucleated in the austenite but with orientations already satisfying a twin relationship. The final, coarsened twin structure is formed as a result that some twins grow and consume their neighbors via twin boundary migration. To understand this interesting behavior, we first analyze lattice transformation in detail with the colored, pre-selected {110} planes of the B2 lattice, and the result is shown in Fig. 8.

In Fig. 8, a region contains the twin boundary in Fig. 4d is magnified, however, the color patterns of the pre-selected {110}

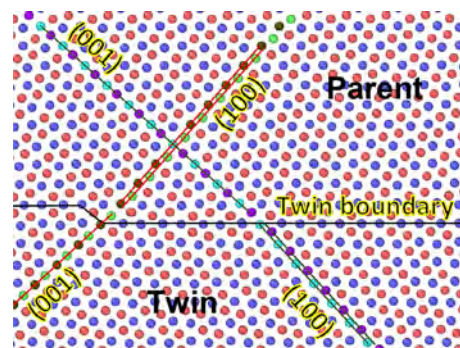


Fig. 8. Lattice transformation analysis for (011) twinning. For convenience, the top crystal is designated as "parent" and the bottom crystal as "twin". The lattice transformation is such that the pre-selected (001) plane of parent (atoms in cyan and purple denoted by the single dark green line) is transformed to the (100) plane of twin, and the pre-selected (100) plane of parent (atoms in light green and dark green denoted by the double red lines) is transformed to the (001) plane of twin. This lattice transformation is very similar to the lattice transformation of {10 $\bar{1}$ 2} twinning in HCP metals which only involves atomic shuffles. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

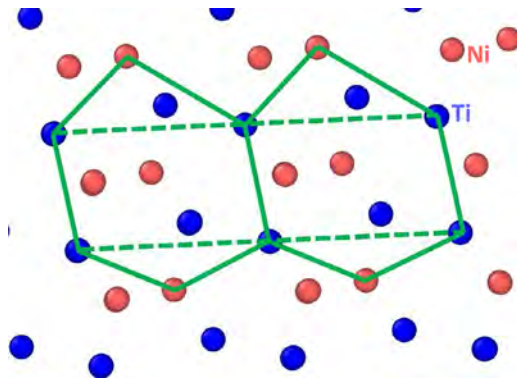


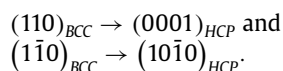
Fig. 9. The martensite variant at the bottom of Fig. 6 is tilted such that the viewing direction is along the [001], i.e. the *c*-axis. The solid green lines connect the atoms on the (001) plane such that distorted hexagons can be constructed. The dashed lines delineate the B19' unit cells. The structure has ...ABABAB... stacking sequence along the [001] (see Fig. 5). Thus, the monoclinic structure can be treated as a distorted HCP structure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

planes are turned on. For the convenience of discussion, the top grain is designated as parent and the bottom grain as twin. Two pre-selected planes are revealed in this plot: one contains atoms in cyan and purple and this is the initial (110) plane of B2, and the other contains atoms in bright green and dark green and this is the initial ($\bar{1}\bar{1}0$) plane of B2. After martensitic transformation, these pre-selected planes of B2 austenite are transformed to the corresponding planes of martensite. It can be seen that the (110) plane of B2 has transformed to the (001) plane of the monoclinic parent, and the ($\bar{1}\bar{1}0$) plane has transformed to the (001) plane of the monoclinic twin.

Another very important lattice transformation is also revealed in this plot. Across the twin boundary, the single layered (001) of the parent has transformed to the double-layered (100) plane of the twin, and the double-layered (100) plane of the parent has transformed to the single-layered (001) plane of the twin. This lattice transformation in twinning is reminiscent of $\{10\bar{1}2\}$ twinning mode in HCP metals. Obviously, atomic shuffles must be involved for this (011) twinning mode in B19' martensite.

Having said that the (011) twinning in B19' monoclinic structure is similar to $\{10\bar{1}2\}$ twinning in HCP metals, we now examine the atomic structure of the (001) plane of martensite and its stacking in real lattice space. Fig. 9 is the plot of (001) plane when the lattice of one of the twins in Fig. 8 is tilted such that the viewing direction is exactly along the [001]. If we connect those atoms with a spacing close to *a* (one of the three parameters of the monoclinic unit lattice), a distorted HCP lattice can be constructed. The stacking sequence of the (001) planes along the *c*-[001] direction is exactly ...ABABAB... which is the stacking sequence of HCP crystals. The dashed lines and the two *a*-axes constitute the (001) face of the monoclinic unit cell. The convenience of treating monoclinic structure as distorted HCP will be shown in the following analysis.

The mechanism of BCC $\rightarrow$ HCP phase transformation was resolved recently [54]. It was shown that, the BCC $\rightarrow$ HCP transformation in pure Ti is accomplished by the lattice transformation that can be described as:



Therefore, one of the two orthogonal $\{110\}$ planes of the BCC is transformed to the basal plane of the HCP, and the other is transformed to the prismatic plane of the HCP. This transformation gives rise to the well-known Burgers orientation relationship (OR) [55]. Because these corresponding planes are parallel to each other, this

lattice transformation only involves atomic shuffles and no homogeneous shear should occur, for the reason that any homogeneous shear would destroy these parallelisms. This mechanism turns out to be applicable for the B2 $\rightarrow$ B19' martensitic transformation, as shown below when we treat monoclinic B19' as a distorted HCP.

We start our analyses with the initial, perfect B2 crystal structure. As shown in Fig. 10a, the initial B2 structure before the simulation started is viewed along the $[1\bar{1}0]$ direction. Without moving any atoms, we construct a hexagon directly from the (110) plane. Of course, this hexagon is not a perfect hexagonal structure but it contains the base structure of one of the faces of the orthorhombic lattice unit which will later transform to the (001) plane of the monoclinic lattice. Repeating this constructing process produces a hexagonal lattice in 3D, as shown in Fig. 10b which is exactly the same structure as Fig. 10a but only slightly tilted. In Fig. 10a, a new coordinate system is defined with the *a*-axis and *b*-axis are the two sides of the front rectangle. In this new coordinate system, the green plane which is one of the two diagonal planes (the shaded plane) has an index of (011). In the representation of the hexagonal lattice, the (011) has a Miller-Bravais index of $\{10\bar{1}2\}$.

Fig. 10a–b show clearly that a hexagonal lattice, although not perfect (it can become perfect if atoms are shuffled to the correct positions and this is exactly BCC $\rightarrow$ HCP phase transformation), can be constructed from the B2 lattice. However, due to the symmetry of the B2 structure, we can construct another hexagonal lattice exactly the same way but in a different orientation. This is shown in Fig. 10c. A new hexagonal lattice which is 90° away from that in Fig. 10b is constructed without moving any atoms of the B2 structure. Again, the same orthorhombic portion of the hexagonal lattice constitutes the base structure of the monoclinic lattice of martensite but with a twin relationship with the one constructed in Fig. 10b.

To show the twin relationship between the two constructed hexagonal lattices, we combine Fig. 10b and c into one plot, as shown in Fig. 10d. So far no atoms are moved during the construction, so the structure is essentially still the B2 austenite. Now it is clearly revealed that the light green plane (011) is perfectly shared by the two constructed hexagonal lattices. In the hexagonal representation, this plane is simply the twinning plane of $\{10\bar{1}2\}$ twinning mode which is the most important twinning mode in all HCP metals [56–59]. In the representation of the orthorhombic or monoclinic structure, this plane is the twinning plane of the martensite. The martensite variants have two possible twinning planes: (011) and (01 $\bar{1}$). Thus, for a B2 lattice, there are 3 pairs of orthogonal $\{011\}$ planes, and each of these $\{011\}$ planes corresponds to a pair of martensite twin variants, giving rise to a total of 6 pairs of martensite twin variants.

The above analysis explains well why in the simulation results (Figs. 4–7), martensite grains are nucleated in a coupled or twinned fashion. When one grain is nucleated, other grains are nucleated in the adjacent regions and are already in $\{011\}$ twin relationship with the first grain. These grains form a twinned martensite structure. Therefore, the twins are actually grains that are nucleated from the B2 austenite but already have a twin relationship. The twin boundaries are highly mobile (see analysis below) and this leads to coalescence and coarsening of one twin at the expense of the other. It is obvious that such a twinned configuration is most effective and efficient to minimize the macroscopic shape strain of the system produced by the martensitic transformation. This effect has been called “self-accommodation” [60–62]. This is seen in Fig. 2 in which the overall shape of the system remains roughly rectangular despite the surface relief and distortion; however, inside the system, numerous small martensite grains are formed with a low symmetry monoclinic structure. If most of the grains were oriented in the same orientation, the

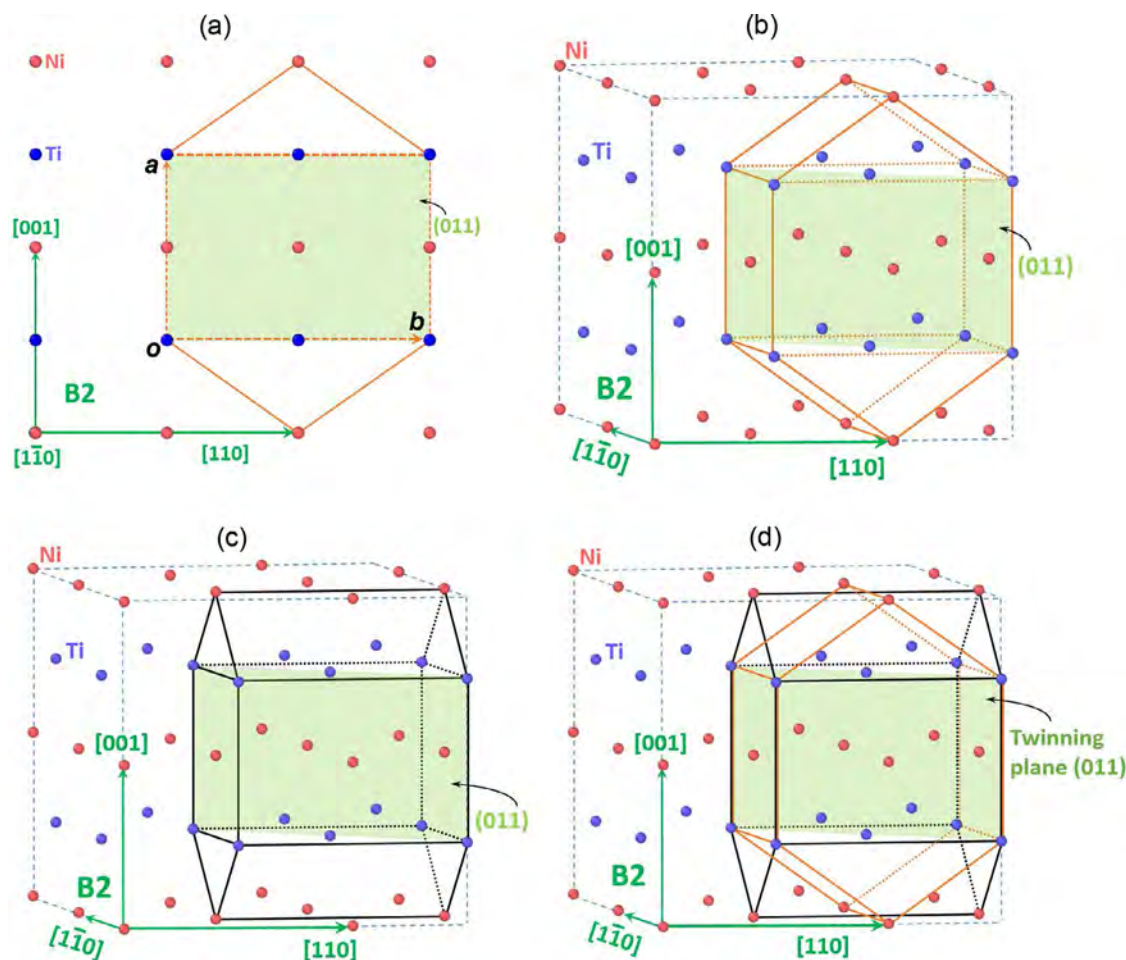


Fig. 10. Crystallography and lattice transformation analysis for B2 $\rightarrow$ B19' transformation and {011} twinning in B19'. (a) A perfect B2 structure when viewed along $[1\bar{1}0]$. A hexagon is constructed by connecting atoms on the $[1\bar{1}0]$ planes. The dashed brown lines delineate an orthorhombic lattice with three axes a , b and c (c is perpendicular to the figure plane). This orthorhombic lattice is the base structure of the B19' martensite. (b) 3D view of (a) by slightly tilting (a). The shaded diagonal plane is (011) with respect to the hexagonal lattice. With respect to the orthorhombic lattice, it is one of the $\{10\bar{1}2\}$, the most important twinning plane of HCP crystals. (c) Another hexagonal lattice can be constructed from the B2 lattice without changing anything. (d) When (b) and (c) are combined, a twinned structure can be seen, in which the shaded plane (011) is the twinning plane. In other words, the two hexagonal lattices satisfy $\{10\bar{1}2\}$ twin relationship. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

overall shape strain would be large. The above analysis also indicates that the B2 $\rightarrow$ B19' martensitic transformation is solely mediated by atomic shuffling, and thus such a transformation is elastic (or dislocation-free) and reversible. If dislocations were involved at the interfaces, the reversibility of migration of these interfaces would be very difficult, if not impossible. This is because, although a dislocation is able to glide backwards for whatever reason, to reverse a whole transformed region back to untransformed structure, all the interfacial dislocations would have to be reversed. If the motion of the dislocations was impeded by other defects, the reversal would be hindered and become very difficult.

4.2. Lattice transformation in twinning in B19' martensite

The simulation results of growth and coalescence of martensite grains (Figs. 4–7) shows with clarity that the interface between two martensite twins are highly mobile even though no external shear strain was applied. The fact that the strain produced during mechanical loading on martensite is reversible or pseudoelastic implies that the migration of the twin boundaries should involve no dislocation-mediated shearing at the interface, otherwise the reversible migration would be very difficult. In the following, we analyze the lattice transformation in twinning in B19' marten-

site. The analyses are illustrated in the representation of distorted HCP lattice for the B19' martensite, for the sake of convenience and clarity.

The analyses were conducted by taking out 17 atoms from a martensite grain (Fig. 11). The positions of these atoms were tracked throughout the simulation. Fig. 11a and b are the initial configuration of these pre-selected atoms, which constitute the hexagonal lattice of the B2 austenite before the martensitic transformation took place. Fig. 11c and d show the final configuration of these 17 atoms after the austenite transformed to the martensite. Detailed evolution of the configuration during martensitic transformation can be found in Video_1 of Supplemental Materials. In Fig. 11a, the shaded planes, i.e. (110), $(1\bar{1}0)$ and (001) of the B2 lattice enclose the orthorhombic lattice inside the hexagonal lattice. If we tilt Fig. 11a such that the viewing direction is exactly along the $[110]$, the projection view of the (110) plane is produced, which is the basal plane of the distorted HCP lattice.

After B2 $\rightarrow$ B19' martensitic transformation, the configuration of the same 17 atoms has changed to the structure in Fig. 11c and d. The distorted HCP lattice (Fig. 11c) remains close to that of the B2 austenite (Fig. 11a), however, the positions of atoms on the middle basal plane in Fig. 11a have shifted and this change can readily be seen in Fig. 11d. The atomic shuffles involved in the martensitic

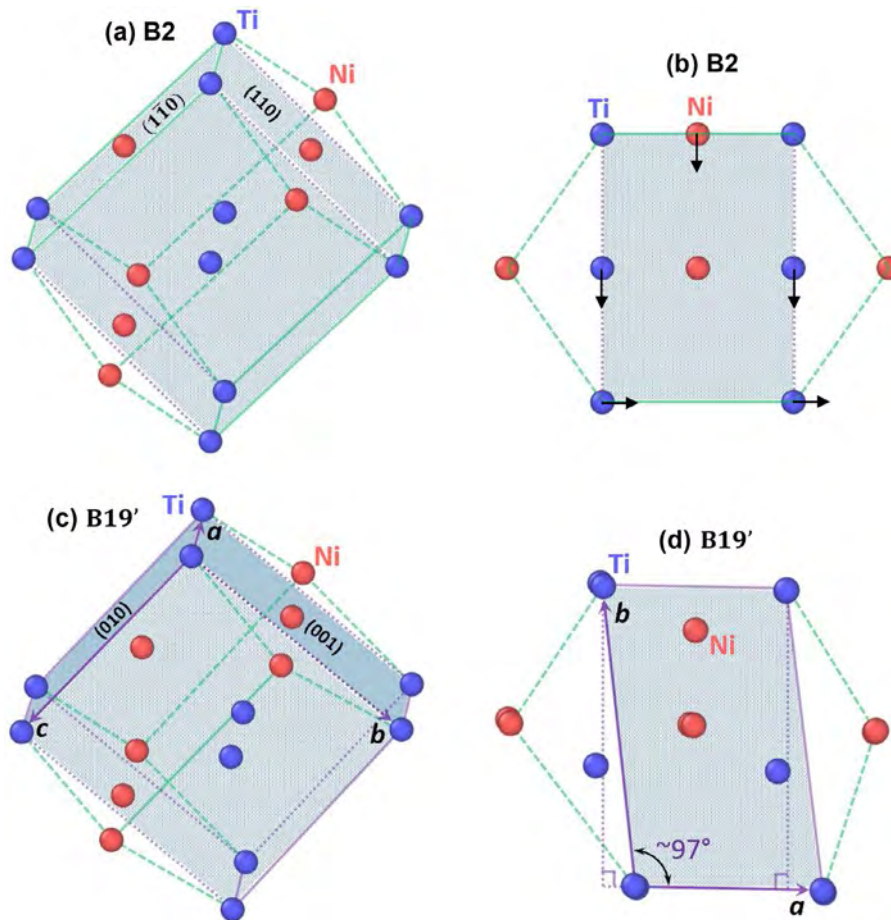


Fig. 11. Lattice correspondence analysis based on the simulation results. A total of 17 atoms are taken out from a martensite grain and plotted. (a) The initial B2 structure is represented as a hexagonal structure before martensitic transformation. The viewing direction is the $[001]$ of B2. The shaded planes enclose the base structure of the monoclinic unit cell for martensite. (b) The B2 structure in (a) when viewed along the $[110]$ of B2. (c) The distorted HCP structure after $B2 \rightarrow B19'$ martensitic transformation. The shaded planes enclose the B19' unit cell. (d) The martensite structure in (c) when viewed along the c -axis of B19'. The structure can be treated as a distorted HCP structure. The monoclinic structure can be seen.

transformation are indicated by the black arrows in Fig. 11b. There are two major shuffles: one is that the three atoms on the middle basal plane shuffle downward toward the center of the triangles of the bottom basal plane; and the other is that the two Ti atoms on the bottom shuffle to the right and this generates the correct lattice parameters of the monoclinic lattice and the angle between the a -axis and the b -axis (close to 97°). It is important to note that the two Ti atoms on the bottom can also shuffle to the left and this would generate an equivalent monoclinic lattice. Without the shuffles of the two Ti atoms on the bottom, a perfect HCP lattice would be created and this is exactly the $BCC \rightarrow HCP$ phase transformation. The lattice transformation in Fig. 11 is the same as that in Fig. 3.

Given the distorted HCP representation of B19' martensite, we can now readily illustrate the two twinning planes in the monoclinic lattice and this is shown in Fig. 12. The atomic configuration is the same as that in Fig. 11c but the front face of the monoclinic unit is removed. The dotted, blue lines delineate the two possible twinning planes, i.e. (011) and $(0\bar{1}\bar{1})$. If we use Miller-Bravais index, these two twinning planes are simply of $\{10\bar{1}2\}$ twinning mode that has been extensively observed in HCP structures [57–59,63].

Next, we analyze the lattice transformation during twin boundary migration of B19' twins. To perform this analysis, atoms of a martensite grain that was eventually consumed by its neighbor were selected and tracked from the beginning until martensitic transformation and subsequent coalescence were finished. The

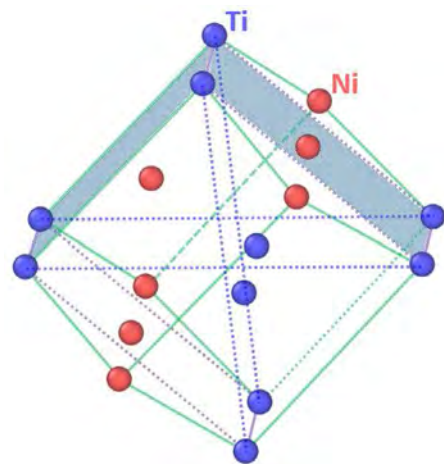


Fig. 12. There are two possible twinning planes (011) and $(0\bar{1}\bar{1})$ for the B19' martensite lattice, as indicated by the blue dotted lines. The shaded planes are the faces of the monoclinic unit cell (see Fig. 11). In the distorted HCP representation, these twinning planes are exactly of the $\{10\bar{1}2\}$ twinning mode that is the most common mode in HCP metals. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

analysis is shown in Fig. 13. More details for the lattice transformation during martensitic transformation and twinning can be found in Video_2 of Supplemental Materials. The viewing direction for the B2 lattice is along the $[001]$ in terms of the BCC unit cell, and

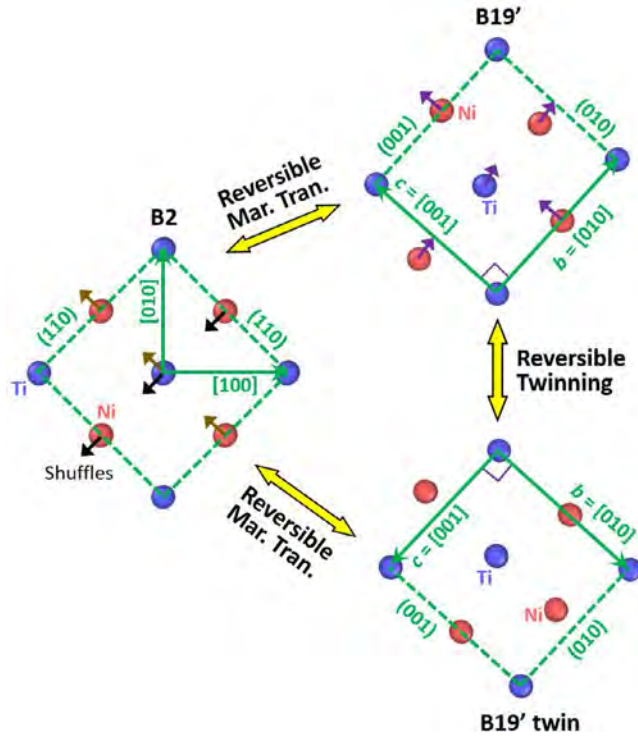


Fig. 13. Lattice transformations between B2, B19' and B19' twin. A group of atoms are selected and plotted in the initial B2, the monoclinic B19', and the twinned B19'. The black arrows indicate the major atomic shuffles that have to be involved for $B2 \rightarrow B19'$, and only atomic shuffles are needed to transform the B2 lattice to the B19' monoclinic lattice. If the atoms of B2 shuffle along the dark brown arrows, then the B2 austenite is transformed to another martensite variant which is the B19' twin. But these two martensite lattices are already in {011} twin relationship. The purple arrows in the B19' indicate the shuffles that are needed to transform the B19' lattice to the B19' twin lattice. All these lattice transformations only involve atomic shuffles and hence are reversible. A 3D view of the lattice transformation for twinning is shown in Fig. 14. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the viewing direction for the B19' martensite is along the [100] in terms of the monoclinic unit cell, but they are nearly parallel. If we compare the structure of the B2 austenite and the B19' martensite, it can be seen that the atomic shuffles (indicated by the black arrows in the B2), along with other shuffles that are not shown transforms the $(110)_{B2}$ to the $(010)_{B19'}$, and the $(\bar{1}\bar{1}0)_{B2}$ to the $(001)_{B19'}$. But if the shuffles are along the dark brown arrows in the B2, then the martensitic transformation would be along the other pathway and generate a different B19' variant which is a twin to the first variant. If we compare the lattice structure of the twins, it can readily be seen that, complex shuffles are involved as indicated by the purple arrows in the B19' lattice. These shuffles transform the $(010)_{B19'}$ to the $(001)_{B19' \text{ twin}}$, and the $(001)_{B19'}$ to the $(010)_{B19' \text{ twin}}$, respectively. This {011} twinning reorients the (001) plane of a martensite variant by $\sim 84^\circ$.

In the following, we show that the (011) twinning process does not involve a homogeneous shear on the twinning plane, and only atomic shuffles are involved. The twinning process described in Fig. 13 can be expressed as:

$$(010)_{B19'} \rightarrow (001)_{B19' \text{ twin}} \text{ and} \\ (001)_{B19'} \rightarrow (010)_{B19' \text{ twin}}$$

But in the HCP representation, these transformations can be expressed as:

$$(10\bar{1}0)_{B19'} \rightarrow (0001)_{B19' \text{ twin}} \text{ and} \\ (0001)_{B19'} \rightarrow (10\bar{1}0)_{B19' \text{ twin}}$$

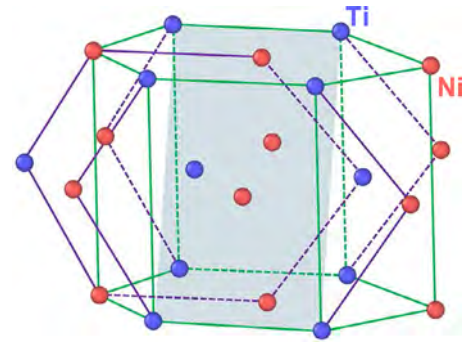


Fig. 14. Lattice transformation in (011) twinning of B19' monoclinic structure, represented in distorted HCP. If the green lattice of the distorted HCP is designated as "parent", then a purple "twin" lattice can be directly constructed from the parent without involving any shear. The lattice transformation is accomplished by the transformation of (001) plane (i.e. the "basal" plane of the green lattice) to the (010) plane (i.e. the "prismatic" plane of the purple lattice); and the transformation of the (010) plane (i.e. the "prismatic" plane of the green lattice) to the (001) plane (i.e. the "basal" plane of the purple lattice). The twinning plane of the two lattices is the shaded (011) (i.e. the {1012} plane of the distorted HCP lattices) which is common to both martensite lattices. This lattice transformation is exactly the same as the crystallographic analysis in Figure 10. Atomic shuffles are all that is needed for the lattice transformation and no homogeneous shear can occur because the shaded twinning plane cannot retain invariant during lattice transformation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Now we translate these lattice transformations into a 3D representation of HCP lattice. We select 23 atoms from the simulation after the B2 austenite has transformed to the B19' martensite, and the configuration is shown in Fig. 14. As displayed in Figs. 10–12, the monoclinic structure can be treated as a distorted HCP structure. We connect and delineate the distorted HCP with solid and dashed green lines. For convenience, we designate this green lattice of distorted HCP as "parent". Without moving any atoms of the parent, a purple lattice can be directly constructed from the parent without involving any shear. The green lattice and the purple lattice naturally satisfy a twin relationship because the shaded plane is perfectly shared by both lattices (cf. Fig. 10d), and the shaded plane is simply the (011) twinning plane of the monoclinic B19' lattice. However, the basal plane of the purple lattice, i.e. the twin, is not single-layered, thus, atomic shuffles have to be involved to make the basal plane single-layered. On the other hand, the prismatic plane of the purple lattice is not double-layered; instead, it is single-layered. Thus, atomic shuffles have to be involved to make the prismatic plane of the purple lattice double-layered (cf. Fig. 13). The transformations can be described as:

$$Basal_{parent} \rightarrow Prismatic_{twin} \text{ and} \\ Prismatic_{parent} \rightarrow Basal_{twin}$$

This lattice transformation is exactly the twinning mechanism for {1012} mode in HCP metals. The required atomic shuffles will destroy the structure of the shaded twinning plane. Thus, the shaded twinning plane cannot remain invariant during twinning. In classical twinning theory, an invariant plane is such a plane on which a homogeneous shear occurs, and its structure must remain invariant, i.e. no distortion should occur to this plane during twin boundary migration. Therefore, the invariant plane strain condition for twinning is not satisfied.

The $Basal_{parent} \rightarrow Prismatic_{twin}$ and $Prismatic_{parent} \rightarrow Basal_{twin}$ transformations, when expressed in terms of the monoclinic lattice, simply are:

$$(001)_{parent} \rightarrow (010)_{twin} \text{ and} \\ (010)_{parent} \rightarrow (001)_{twin}$$

Table 1
Twinning modes in distorted hexagonal indices.

In monoclinic index	In distorted HCP index
(011)	{10 $\bar{1}$ 2}
(111)	{10 $\bar{1}$ 1}
(001)	(0001)
(100)	{11 $\bar{2}$ 0}
(010)	{10 $\bar{1}$ 0}
(20 $\bar{1}$)	{11 $\bar{2}$ 1}
(101) (unreported)	{11 $\bar{2}$ 2}

And this is exactly the twinning mechanism shown in Figs. 10 and 13. Therefore, atomic shuffles are all that is needed for the lattice transformation and no homogeneous shear can occur on the twinning plane because the twinning plane cannot be retained invariant during lattice transformation. Because no homogeneous shear is involved on the twinning plane, this twinning mechanism involves no twinning dislocations and hence is reversible. This is obviously seen in Fig. 14 the parent and the twin lattices can interchange, and the critical stress for activating (011) twinning in B19' martensite can be very low because no shear is involved. In fact, {10 $\bar{1}$ 2} twinning in HCP metals such as Mg, Ti and Co etc. is one of the easiest deformation mode. In pure Mg, the critical resolved shear stress (CRSS) for {10 $\bar{1}$ 2} twinning is on the order of ~ 10 MPa [64]. In highly textured Mg alloys, {10 $\bar{1}$ 2} twins dominate the low stress stage deformation when a tensile load is applied along the *c*-axis of individual grains [65–67]. Once {10 $\bar{1}$ 2} twins are formed, they are able to engulf dislocations and precipitates and consume whole grain [68,69]. Importantly, {10 $\bar{1}$ 2} twinning has been found reversible in extensive experiments [70,71].

The above analyses demonstrate that all the lattice transformations in B2 $\rightarrow$ B19' phase transition and {011} twinning in martensite only require atomic shuffles and involve no interfacial dislocations, so they are all reversible.

In our simulation results, only {011} twinning mode was observed and no other twinning modes were present. This is also true in our simulations when martensite is deformed (not shown). It is now worth re-examining the twinning modes that were proposed in previous works by converting the Miller indices with respect to the monoclinic coordinates into the Miller-Bravais indices with respect to the distorted HCP coordinates. The conversion is shown in Table 1. For the (111) mode, it corresponds to the {10 $\bar{1}$ 1} mode of HCP metals. This twinning mode is called “contraction twinning” for metals with *c/a* less than $\sqrt{3}$ [72]. This twinning mode is much less common than {10 $\bar{1}$ 2} mode. It involves a homogeneous shear which is mediated by zonal twinning dislocations, as well as large shuffles [73,74]. Thus, reversible twinning for this mode is difficult. For the (20 $\bar{1}$) mode, it corresponds to the {11 $\bar{2}$ 1} mode of HCP metals, which is not a common twinning mode either. The interplanar spacing of the {11 $\bar{2}$ 1} twinning plane is very small, indicating that this twinning mode may be difficult to activate. For the reported (001) mode, it corresponds to the basal plane of the distorted HCP lattice. As pointed out by Knowles and Smith [19], it is unable to produce the lattice invariant shear. Thus, it is more likely to be a slip system, but more calculations and experimental observations are needed to verify this conclusion. For the reported (100) mode, it corresponds to the (11 $\bar{2}$ 0) plane which is neither a twinning plane nor a slip plane. For the (101) mode which was not mentioned in the literature, it corresponds to the {11 $\bar{2}$ 2} twinning mode which was observed in Ti and Zr [56]. This twinning mode is important when HCP crystals are compressed

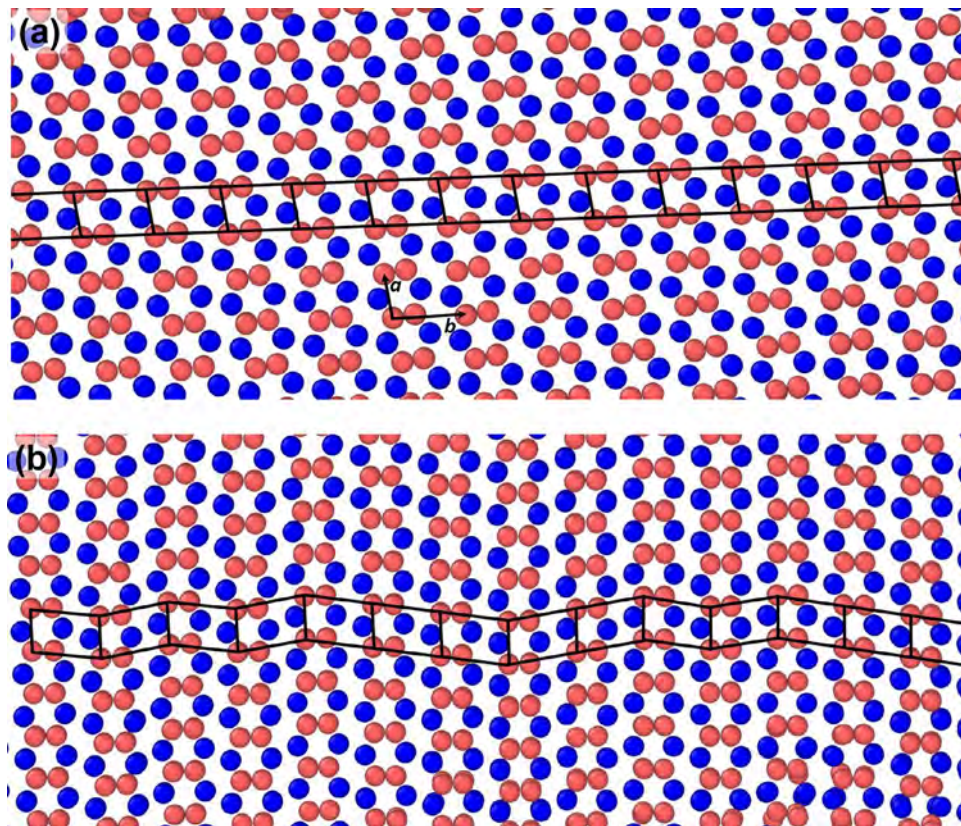


Fig. 15. Dual-lattice structure of monoclinic B19' martensite. Ni atoms are in red and Ti in blue. (a) The martensite single crystal has a perfect monoclinic lattice in real space. (b) The martensite single crystal has dual lattices that orient either up or down. In sharp contrast to (a), no long range periodicity in real space can be defined. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

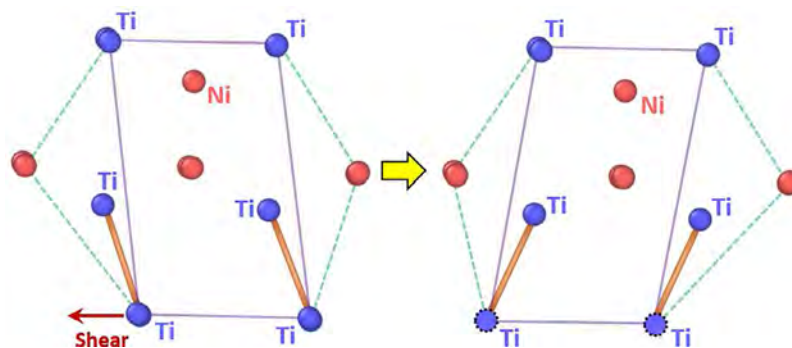


Fig. 16. Mechanism for the formation of the dual-lattice structure in the B19' martensite. The weak Ti-Ti bonds (indicated by the brown bold lines) can be sheared from right to left, forming a monoclinic B19' lattice identical to the original lattice but oriented differently (minor shuffles may be involved). This mechanism provides the monoclinic martensite an extra degree of freedom to be very adaptive to external and internal strains. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

along the c -axis. For the (010) mode, this is a special plane with a unique structure and more detailed discussion is provided below.

4.3. Dual-lattice structure in B19' martensite

Our simulation also reveals a very interesting structure in B19' martensite – some martensite variants present a dual-lattice structure. Fig. 15a shows a magnified view of a portion of the martensite grain close to the bottom surface (see Fig. 6). This structure is a perfect a monoclinic structure of B19'. The viewing direction is along the [001], i.e. the (001) plane of the monoclinic units is seen. The units are delineated by the black lines with the a -axis and b -axis are marked out. However, not all the martensite grains have this structure.

In stark contrast, the martensite grain near the top surface (see Fig. 6) has a very special structure, as shown in Fig. 15b. The black lines delineate lattice units of the monoclinic B19' martensite. It can be seen that the lattice units are not aligned in the same direction. Locally, some neighboring units form a v-shaped or Λ -shaped pattern. Some local units do present a periodicity but only in a short range and the number of repeating units varies. Overall, no long range periodicity in real space can be defined. This structure was described as another “twinned structure” in B19' martensite in the literature [75].

Although the v-shaped or the Λ -shaped patterns of lattice units seemingly appear to be a twinned structure, careful examination of the atomic structure of the “twinning plane” reveals that this is not the case. If they were twinned structures, the “twinning plane” would be the (010) plane. But it can be seen from the geometry that the (010) planes cannot be a twinning plane, because a homogeneous shear on these planes does not produce twin symmetry about the slip plane. On the other hand, the interfaces between these subdomains are perfectly coherent and they are mobile (see below). In this regard, we define this unique atomic structure “dual-lattice structure”, meaning that two differently oriented but structurally equivalent lattices co-exist in a single crystal. Then how is this very special dual-lattice structure formed in our simulations?

As mentioned above and shown in Fig. 11b and d, during formation of the monoclinic structure, the Ti atoms on the bottom (Fig. 11d) also have a chance to move to the left, forming an almost identical monoclinic structure but with a different orientation. This process is shown in Fig. 16. The Ti-Ti bonds (indicated by the bold brown lines) can swing their positions around the c -axis and reach the positions indicated by the dotted circles. The swap of positions of the Ti atoms between the two structures forms the v-shaped or the Λ -shaped configurations of lattice units in Fig. 15b. Such swap can occur when internal strain or external

strain (for instance, the shear strain indicated by the red arrow) or both have to be accommodated during thermally activated or stress-induced martensitic transformation. This unique property of monoclinic B19' martensite provides an extra degree of freedom to reduce the overall shape strain and accommodate internal and external strains, rendering the B19' structure extremely adaptive to straining. It is interesting to note that the dual-lattice structure of martensite can be regarded as another type of “adaptive martensite”, a concept discussed by Niemann et al. [76]. In this concept, the martensite assumes a modulated structure that is composed of twins whose lamellar thickness is dependent of the twin boundary energy. Such interfacial energy is counterbalanced by the reduction in strain energy generated by martensitic transformation. We will present elsewhere detailed energy calculations for such interesting deformation, as well as how a single crystal B19' martensite responds to various straining conditions.

5. Conclusions

In this work, we performed atomistic simulations of martensitic transformation in NiTi shape memory alloy, and detailed analyses on lattice transformation in phase transition and formation of twins in martensite. The following conclusions can be reached.

- (1) The mechanism for B2 $\rightarrow$ B19' martensitic transformation is essentially the same as that for BCC $\rightarrow$ HCP phase transformation, if the monoclinic crystal structure of martensite is treated as a distorted HCP structure. Such a treatment connects well the phase transformation mechanism and twinning mechanism in B2 $\rightarrow$ B19' with the mechanisms in higher symmetry structures that are relatively better understood. Our analyses explain well why martensitic transformation in NiTi is reversible and the reversibility originates from the fact that only atomic shuffles are involved in the phase transformation. Thus, the inter-phase boundaries are elastic and dislocation-free.
- (2) Martensite grains are nucleated in paired fashion directly from the austenite. Pairs of variants are already in twin relationship and self-accommodation is naturally achieved. The twinning mechanism in monoclinic martensite is essentially the same as {10 $\bar{1}$ 2} twinning mode which is the most common in HCP metals. This twinning mode also only involves atomic shuffles and no interfacial dislocations are involved. Thus, the twin boundaries are elastic and their migration is also reversible. Once nucleated, some martensite variants grow at the expense of other variants, eventually a coarsened twin structure is formed.
- (3) A very special, dual-lattice structure was discovered in B19' martensite. The relatively weak Ti-Ti bonds in the monoclinic unit cell can swap position under a shear stress or strain, lead-

ing to locally changed lattice orientation in a single martensite grain. Such a special structure provides an extra degree of freedom for the martensite to accommodate external strain.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.actamat.2020.08.039](https://doi.org/10.1016/j.actamat.2020.08.039).

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