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Transformation-induced Plasticity in Omega Titanium

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 ω -titanium (Ti) is a high-pressure phase that is conventionally perceived to be brittle and nondeformable, although direct investigations of its deformation process remain scarce. In this work, we perform molecular dynamics simulations to study the deformation process of ω -Ti with initial defects and find that stress-induced $\omega \rightarrow \alpha$ martensitic transformation can cause extensive plasticity in ω -Ti under various loading directions. Moreover, for the first time, we demonstrate that four types of transformation twins— $\{11\overline{2}1\}$, $\{11\overline{2}2\}$, $\{10\bar{1}2\}$, and $\{10\bar{1}1\}$ twins—can be formed through the $\omega \rightarrow \alpha$ martensitic phase transformation. This work advances the understanding of plastic deformation in ω -Ti and unveils the essential role of the metastable ω -phase in the formation of transformation twins.

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I. INTRODUCTION

Extensive research efforts have been devoted to titanium (Ti) and its alloys due to their high strength-to-weight ratio and extraordinary high-temperature performance^{1–3}. At ambient conditions, Ti prefers to exist in hexagonal close-packed (hcp or α) phase, while it can transform into ω -phase at high pressures or into body-centered cubic (bcc or β) phase at high temperatures (around 1,100 K). The ω -phase can be obtained under high pressure or shock loading experiments because the high pressure can modify the electronic band structure and stabilize the ω -phase⁴. In addition, alloying with d-rich transition metal elements, such as vanadium and niobium, can also stabilize the ω -phase⁴.

Since its discovery in 1954⁵, ω -phase has received extensive interest because of its profound effect on the mechanical properties of Ti alloys^{6,7}. The ω -phase has an A1B₂ structure and contains three atoms in the primitive unit cell, with one atom in the A-plane and two atoms in the B-plane. In particular, the A- and B-planes have different bonding properties: A-planes are purely metallic, like hcp and bcc Ti, while B-planes have certain covalent nature⁴. These peculiar properties were believed to cause the brittleness of the ω -phase. Thus, ω -phase is commonly used as a precipitation-hardening mechanism to enhance the strength and microhardness of Ti alloys, though a large number of the ω precipitates can deteriorate the ductility of the alloys^{8,9}.

Studies directly investigating the physical properties of ω -phase are scarce^{7,10,11}, because ω -phase usually exists as nanosized precipitates in Ti alloys and was only recently obtained in the bulk form¹². In 2013, Tane et al. investigated the elastic properties of ω -Ti produced by high-pressure torsion¹⁰. They found ω -Ti has higher Young's modulus and shear modulus than the β -and α -phases, though the plastic deformation in ω -phase remained unexplored. As an attempt to investigate the plastic deformation, Kumar et al. calculated the generalized stacking fault energy surfaces using density-functional theory, through which they identified the favored slip modes in the ω -Ti as prismatic $\langle c \rangle$, prismatic-II [10 $\bar{1}$ 0], and pyramidal-II $\langle c+a \rangle^7$. Their density-functional theory calculation quantifies the relative ease of different slip systems, though methods that can handle millions of atoms are still required to study the dynamic process of plastic deformation. Accordingly, Zong et al. performed large-scale molecular dynamics (MD) simulations in single-crystal ω -Ti and found highly anisotropic deformation behavior¹¹. They observed superplastic deformation behavior due to $\omega \rightarrow \alpha$ martensitic phase transformation under [10 $\bar{1}$ 0] compression as well as brittle fracture under [0001] loading. Nonetheless, only pristine single crystal was studied,

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although Ti and its alloys, particularly the ω -Ti^{12,13}, almost always contain considerable initial defects. As demonstrated by our previous work^{14–18}, initial defects can affect the deformation process and mechanical properties of metals significantly. In this work, we strive to systematically investigate the deformation process of quenched ω -Ti with initial defects owing to the omnipresence of ω -Ti in quenched metastable Ti alloys.

Ti and its alloys are well known to form transformation twins as a result of martensitic phase transformation induced by quenching or mechanical strain^{19–22}. Notably, $\{10\bar{1}1\}$ transformation twins were widely reported to form during $\beta \to \alpha$ martensitic phase transformation among a wide range of Ti alloys and pure Ti^{19–21}. Similarly, the metastable ω -phase can transform back to the thermodynamically stable α -phase upon release of the high pressure or heating to around 150° C, and thus may also form transformation twins. For instance, $\{10\bar{1}1\}$ twin was observed to form as a result of $\omega \to \alpha$ martensitic phase transformation in pure Ti¹¹. Accordingly, the objective of this work is to rigorously investigate the deformation of ω -Ti with initial defects under various loading directions and to elucidate the formation mechanism of different transformation twins.

The rest of this paper is organized as follows: Section II describes the methodology of this work and the construction of the quenched ω -Ti structure. In Section III, we present our findings of the transformation-induced plasticity in ω -Ti and the formation mechanisms of transformation twins. Finally, we conclude this paper in Section V.

II. METHODOLOGY

A. MD simulations

In this work, we use the LAMMPS package²³ to perform all the MD simulations with a timestep size of 1 fs. The interactions between Ti atoms are modeled by the embedded-atom method potential developed by Mendelev et al.²⁴. The initial simulation domain is an α -Ti of 29.5 × 25.5 × 24.1 nm^3 (one million atoms) with the periodic boundary condition applied to all three dimensions. At the beginning of the simulation, we assign random atomic velocities following the Gaussian distribution with an average temperature of 10 K. In order to reduce the simulation time required for the melting process and to ensure fully melting of the Ti structure, we heat the structure to a temperature (2266 K) higher than the melting point (1923 K). To achieve complete melting, the simulation domain is maintained at 2,266 K for 500 ps before it is quenched to 10 K.

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Subsequently, we relax the structure at 10 K and 0 Pa in the isothermal-isobaric ensemble using the Nosé-Hoover thermostat²⁵ and the Parrinello-Rahman barostat²⁶ for 100 ps. The ω -phase is predicted by the adopted Mendelev et al.'s²⁴ interatomic potential to only have a slightly higher energy (7 meV/atom) than the α -phase. As a result, the quenching simulation generates an ω -Ti structure, which is stabilized by the fast quenching rate and the abundant internal defects. To study the deformation process, we apply uniaxial loading to the quenched ω -Ti structure with a strain rate of 10^8 s⁻¹. It should be noted that the application of a very high strain rate even on the order of 10¹¹ s⁻¹ in MD simulations is very common^{27–30}. Despite this inherent limitation, previous MD simulations have provided useful guidance or rigorous interpretations to deformation behaviors under realistic. We applied uniaxial loading by changing the simulation box length in the loading direction at a constant strain rate and then remapping the atom coordinates within the modified simulation box. As a result of Poisson's effect, the changes of other two boundaries are naturally incorporated by solving the isothermal-isobaric equations of motion at zero pressure. OVITO³¹ is used to visualize and analyze the microstructure evolution. The common neighbor analysis 32,33 is used to identify the crystal structure, with ω , β , α , and face-centered cubic (fcc) phases denoted in yellow, red, cyan, and green, respectively.

B. Lattice dynamics calculations

In our lattice dynamics calculations, supercells of α (5 × 5 × 5), ω (3 × 3 × 3), and β (4 × 4 × 4), are fully relaxed at zero pressure. The raw second-order force constants are obtained using the central finite difference method and are further adjusted with the linear regression approach (ordinary least-squares) to apply the symmetry constraints [37]. Afterwards, the symmetrized force constants are used to calculate the dynamical matrix, from which we obtain the phonon bandstructure (the phonon eigenvectors and eigenvalues). To ensure the direct correspondence between our lattice dynamics calculations and MD simulations, we use the same cutoff radius and empirical interatomic potential in these two types of calculations/simulations.

III. RESULTS

First, we will describe the deformation process of the ω -Ti structure under six loading conditions. Then, we will analyze the formation mechanisms for each of the five transformation twins

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observed in our MD simulations. Finally, we will discuss the orientation relations of all the α -variants captured by our MD simulations.

A. The radial distribution functions

As shown in Fig. 1a, the quenched Ti structure contains some retained β -phase and traces of α -phase. More specifically, common neighbor analysis reveals that it has 11.8% of β -phase and 2.4% of α -phase initially. It is composed of a predominant grain and a much smaller grain, which is close to a single-crystal ω -Ti. Its ω -phase nature is further confirmed by the radial distribution function (RDF) in Fig. 1b, in which the RDF of the quenched structure displays similar peaks as those of single-crystal ω -phase. Notably, the first three peaks in the RDFs (2.675, 2.825, and 3.025 Å) correspond to the first three nearest neighbours in the ω -phase that are highlighted in the inset of Fig. 1b.

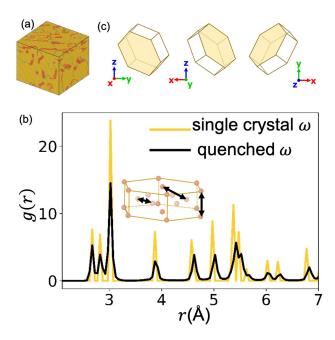


FIG. 1. (a) The quenched ω -Ti structure and (c) its orientation with respect to the x-, y-, and z-axes. The basal plane of the ω unit cell is highlighted in yellow. (b) The comparison of the RDF between the quenched ω -Ti structure and single crystal ω -Ti. The first three peaks of the RDF correspond to the first three nearest neighbours in the ω -phase, of which the atom pairs are connected by the black arrows in the inset.

We study six loading conditions, in each case uniaxial tension or compression is applied along the x-, y-, or z-axis of the simulation domain. The orientation of the initial ω -Ti structure with

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respect to the x-, y-, and z-axes are shown in Fig. 1c. Figure 2 shows the evolution of the RDFs under all six loading conditions, from which we observe the gradual change in the RDF from that of the ω -phase to that of the α -phase. Specifically, with increasing strain, the peaks belonging to the ω -phase broaden owing to the elastic strain and the activation of $\omega \rightarrow \alpha$ martensitic phase transformation. As a result, the second and third peaks merge into one broad peak when the strain reaches 5%. With increasing amount of α -phase, the most prominent peak in the RDF gradually shifts from 3.025 Å of the ω -phase to 2.92 Å of the α -phase. The former is the distance between atoms in the A-plane and atoms in the B-plane of the A1B₂ structure of the ω -phase, while the latter is the distance between two atoms in the basal plane of the α -phase. Notably, the first peak corresponding to the nearest-neighbour distance of 2.675 Å in the ω -phase completely disappears at 20% strain under x-axis compression (Fig. 2a), y-axis compression (Fig. 2c), and z-axis tension(Fig. 2f), suggesting the transformation of almost all the parent ω -phase.

B. The stress-strain curves

To further investigate the phase transformation and plastic deformation quantitatively, we plot the evolution of the percentages of ω -Ti and α -Ti and the stress-strain curves in Fig. 3. The β -phase shows a continuous decreasing trend and a small percentage (<3%) and is thus omitted in Fig. 3. During the elastic regime, we observe a slight increase in the percentage of the ω -phase and a stable small percentage of the α -phase. The former is due to the transformation from the β -phase that is retained from the quenching process. Upon yielding, the $\omega \rightarrow \alpha$ martensitic phase transformation is activated, leading to the most prominent stress drops in the stress-strain curves. The $\omega \rightarrow \alpha$ phase transformation proceeds with increasing applied strain, and, thus, the percentage of ω -Ti keeps decreasing, while that of the α -Ti keeps increasing. In addition, because our initial ω -Ti structure contains defects, the propagating ω - α interfaces can decelerate when they are impeded by the defects and then accelerate again after they bypass the defects. The accelerated ω - α interfaces account for some of the smaller stress drops in the stress-strain curves.

Our MD reveals that the $\omega \rightarrow \alpha$ phase transformation displays different kinetics under different loading directions. Specifically, the phase transformation occurs quickly under x-axis compression (Fig. 3a), y-axis compression (Fig. 3c) and tension (Fig. 3d), and z-axis tension (Fig. 3f), leading to a high percentage of Ti in the form of α -phase (>70%) and a low percentage in the ω -phase (<25%)

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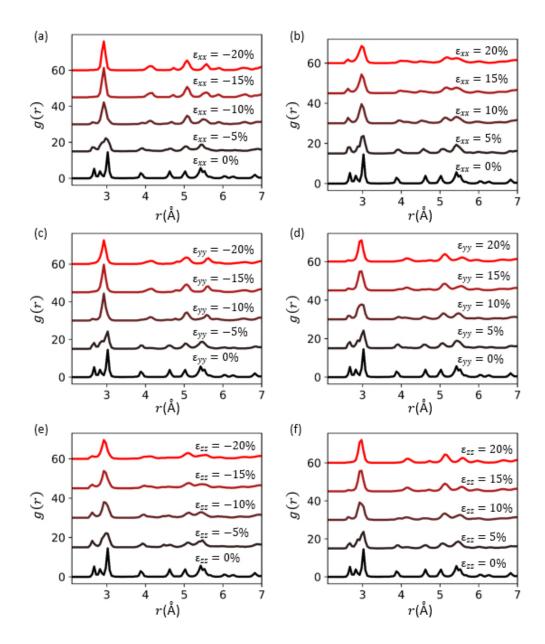


FIG. 2. The evolution of RDFs during the deformation process under (a) x-axis compression, (b) x-axis tension, (c) y-axis compression, (d) y-axis tension, (e) z-axis compression, and (f) z-axis tension.

at the end of the deformation process. In contrast, the phase transformation occurs at a lower speed under x-axis tension (Fig. 3b) and z-axis compression (Fig. 3e), and the final percentages of Ti in the α -phase are only around 50%. This difference can be clearly seen from the microstructures at 10% and 20% strains in the insets of Fig. 3. It should be noted that the ω -phase is identified as amorphous atoms by common neighbor analysis, and thus, the percentage shown in Fig. 3 accounts for both ω -phase and amorphous atoms. A careful examination of the microstructures reveals that

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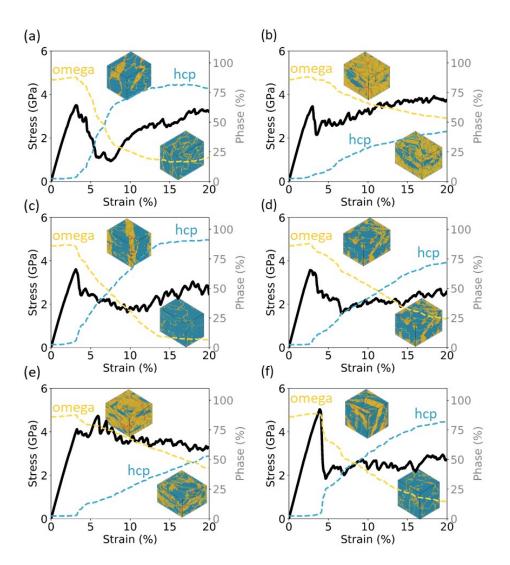


FIG. 3. The stress-strain curves (black lines) and the percentage of ω -Ti (yellow dashed lines) and α -Ti (cyan dashed lines) under (a) x-axis compression, (b) x-axis tension, (c) y-axis compression, (d) y-axis tension, (e) z-axis compression, and (f) z-axis tension. The insets show the corresponding microstructures at 10% and 20% applied strains.

amorphous atoms mostly form at the end of the $\omega \rightarrow \alpha$ phase transformation and are much fewer than the actual ω -phase atoms, because they mainly exist in dislocations and twin boundaries in the newly-formed α -variant.

C. The martensite microstructure

The $\omega \rightarrow \alpha$ phase transformation leads to complex martensite microstructure, including five types of transformation twins. Specifically, we observe $\{11\overline{2}1\}$ twins (Fig. 4a) and $\{10\overline{1}2\}$ twins

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(Fig. 4b) under x-axis compression, $\{11\bar{2}2\}$ twins under y-axis tension (Fig. 4c), $\{10\bar{1}1\}$ twins under x-axis tension (Fig. 4d), and threefold twins under z-axis tension (Fig. 4e). In the threefold twin, three cozone $\{10\bar{1}1\}$ twin boundaries join at a common $\langle 11\bar{2}0\rangle_{\alpha}$ axis, as shown in Fig. 4e. Our simulations under y-axis compression and z-axis compression only reveal a single newlyformed α -phase.

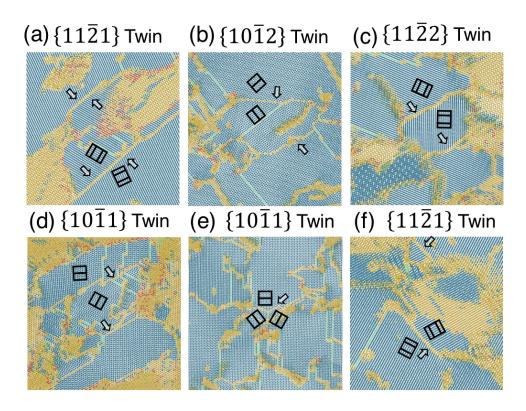


FIG. 4. Slices of the martensite microstructures clearly showing five types of transformation twins formed in our MD simulations under (a-b) x-axis compression, (c) y-axis tension, (d) x-axis tension, and (e) z-axis tension. (f) The simulation of x-axis compression has been verified using another modified embedded atom method potential for Ti^{34} , which also shows the formation of $\{11\bar{2}1\}$ twins.

Previously, only $\{10\overline{1}1\}$ twins were identified as transformation twins in pure Ti, which is caused by temperature-induced $\beta \rightarrow \alpha$ phase transformation¹⁹ or stress-induced $\omega \rightarrow \alpha$ phase transformation¹¹. In this work, we have shown, for the first time, that $\{11\overline{2}1\}$, $\{11\overline{2}2\}$, and $\{10\overline{1}2\}$ twins, as well as the threefold $\{10\overline{1}1\}$ twins, can all be formed through stress-induced $\omega \rightarrow \alpha$ martensitic phase transformation in pure Ti. To rule out the empirical potential dependence of our results, the MD simulation of x-axis compression has been performed using a modified embedded-atom method potential for Ti³⁴, which is carefully designed to capture the $\alpha \leftrightarrow \omega$

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martensitic phase transformation. The MD simulation using the second potential also predicts the formation of $\{11\bar{2}1\}$ twins (Fig. 4f) and $\{10\bar{1}2\}$ twins under x-axis compression, reaffirming our findings.

D. The formation mechanism of various transformation twins

The core of this section is to demonstrate that the afore-discussed dependence of twinning mode on the loading directions is rooted in different orientation relation of $\omega \to \alpha$ martensitic phase transformation. Specifically, we observe two different orientation relations in our MD simulations, in which the correspondence of ω - and α -phases will be discussed in more details in Section IV B. The two orientation relations are the same as Variant I and Variant II in Usikov and Zilbershtein's notation³⁵ and are referred to as OR I and OR II in this paper to avoid any confusion with variant of martensite. Specifically, in OR I, $(0001)_{\alpha} \parallel (01\bar{1}1)_{\omega}$ and $[11\bar{2}0]_{\alpha} \parallel [\bar{1}011]_{\omega}$; in OR II, $(0001)_{\alpha} \parallel (11\bar{2}0)_{\omega}$ and $[11\bar{2}0]_{\alpha} \parallel [0001]_{\omega}$.

As displayed in Fig. 5, the parent ω -phase can transform into two α -variants through two separate OR I and OR II. As a result, different twins are formed owing to the different misorientation angles between the two newly-formed α -variants. As schematically shown in Fig. 5a, two separate OR I—two crystallographically equivalent $\{01\bar{1}1\}_{\omega}$ planes of the parent ω -phase directly transform into the basal planes of two α -variants—can form a $\{11\bar{2}2\}_{\alpha}$ twin. Because these two $\{01\bar{1}1\}_{\omega}$ planes share a common $\langle 11\bar{2}0\rangle_{\omega}$ direction, this process can be clearly demonstrated by the projection of our MD simulation along the common $\langle 11\bar{2}0\rangle_{\omega}$ direction, as shown in Fig. 5b. Under y-axis tension, the left and right regions of the same ω -phase transform into two different α -variants. Upon the merging of the two α -variants, a coherent twin boundary forms in between. The twin boundary shows a misorientation angle of 65° and a three-atom interface structure, matching those of the $\{11\bar{2}2\}$ twin boundary in α -Ti. It should be noted that this twin formation process is possible because the angle between the two $\{01\bar{1}1\}_{\omega}$ planes (63°) is very close to the misorientation angle of the $\{11\bar{2}2\}$ twin (65°) .

Similarly, two separate OR I can form a $\{11\bar{2}1\}$ twin, as schematically shown in Fig. 5c. In this case, the two $\{01\bar{1}1\}_{\omega}$ planes share a common $\langle 11\bar{2}3\rangle_{\omega}$ direction, which differs from the above case of $\{11\bar{2}2\}$ twin. Fig. 5d shows the detailed formation process of the $\{11\bar{2}1\}$ twin in our MD simulation of x-axis compression. The right region of the parent ω -phase transforms into the first α -variant. Subsequently, the second α -variant nucleates at the ω - α interface and

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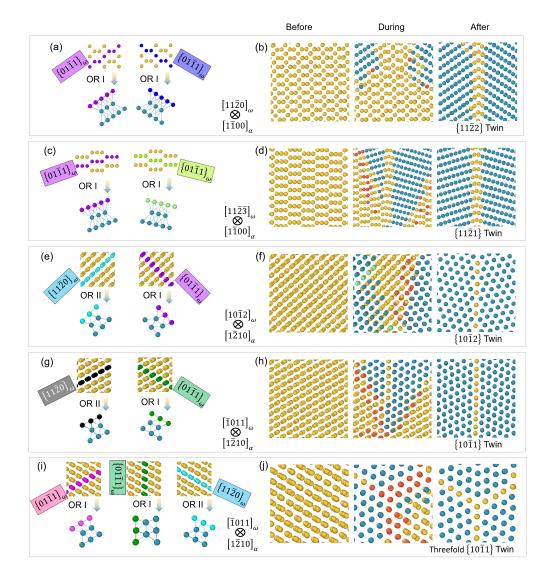


FIG. 5. The formation processes of the five transformation twins in our MD simulations are shown in b, d, f, h, and j, while a, c, e, g, and i are the corresponding schematics. The plane correspondence during the $\omega \rightarrow \alpha$ phase transformation is demonstrated by the highlighting colors. The planes that are highlighted by the same color among different cases are the same plane of the parent ω -phase. The purple, blue, green, dark green, and pink planes are $\{01\bar{1}1\}_{\omega}$ planes; the light blue and black planes are $\{11\bar{2}0\}_{\omega}$ planes.

continues to consume the parent ω -phase, forming a twin boundary with respect to the first α -variant. Obviously, the misorientation of 33° and the alternate three-atom/two-atom interface structure match those of the $\{11\bar{2}1\}$ twin boundary in α -Ti. Similar to the $\{11\bar{2}2\}$ twin, the formation of the $\{11\bar{2}1\}$ twin is made possible by the matching between the misorientation angles of the $\{11\bar{2}1\}$ twin and the two $\{01\bar{1}1\}_{\omega}$ planes involved, as listed in Table I.

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Twin type		{1121}	{1012}	{1011}
Theoretical misorientation angle	65°	35°	85°	57°
Misorientation angle measured in MD	65±1°	33±1°	87±1°	60±1°
The angle between participating ω planes*	63°	32°	90°	60°

TABLE I. The misorientation angles of each transformation twin and the angles between ω planes involved in the twin formation process. The latter is taken as an acute angle to be consistent with the definition of the former. * Calculation based on c/a=0.613 for ω -Ti.

In contrast to the aforementioned two types of twins formed through two separate OR I, the $\{10\bar{1}2\}$ twin is formed through the simultaneous occurrence of OR I and OR II, as schematically shown in Fig. 5e. Figure 5f shows our MD simulation of x-axis compression projected along the $\langle 11\bar{2}0\rangle_{\omega}$ direction. Evidently, the ω - α interface on the right side contains a thin layer of β -phase and follows OR I, while the left ω - α interface follows OR II. The merging of the two newlyformed α -variants results in a coherent $\{10\bar{1}2\}$ twin boundary.

In a different case, the simultaneous occurrence of OR I and OR II can lead to the formation of a $\{10\bar{1}1\}$ twin, as schematically shown in Fig. 5g. Our MD simulation of x-axis tension is projected along the $\langle\bar{1}011\rangle_{\omega}$ direction in Fig. 5h, in which the merging of the two α -variants leads to a coherent $\{10\bar{1}1\}$ twin boundary.

Finally, we note that the simultaneous occurrence of two separate OR I and one OR II can lead to the formation of a threefold $\{10\bar{1}1\}$ twin, as illustrated in Fig. 5i. Our MD simulation of z-axis tension is projected along the $\langle \bar{1}011\rangle_{\omega}$ direction in Fig. 5h, which captures the formation of three cozone $\{10\bar{1}1\}$ twin boundaries adjoining at a common $\langle 11\bar{2}0\rangle_{\alpha}$ axis. Compared to a single $\{10\bar{1}1\}$ twin, the threefold $\{10\bar{1}1\}$ twin can better accommodate the strain associated with the martensitic phase transformation. Similar threefold symmetry has been observed in the martensite microstructure of pure Ti^{22} , Ti alloy²¹, $iron^{36}$, and Ni-Al alloys³⁷.

E. The crystallographic origin of the twin formation process

We note that the formation of all the transformation twins is rooted in the fact that the angles between the crystallographic planes in the ω -phase $(\{01\bar{1}1\}_{\omega} \text{ and/or } \{11\bar{2}0\}_{\omega})$ —which can directly transform into the basal planes of the α -variants—are close to the misorientation angles of the twins. The relevant values are summarized in Table I.

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Furthermore, we emphasize that the α -variants—that constitute the five types of transformation twins are not completely independent—as they can be involved in more than one type of twins. As shown in Fig. 5, the planes highlighted in purple are involved in multiple twins, so are the planes highlighted in dark green and light blue. Theoretically, there are six $\{01\bar{1}1\}_{\omega}$ planes and three $\{11\bar{2}0\}_{\omega}$ planes in the parent ω -phase. The direct transformation of these planes to basal planes of the α -variants can lead to the formation of a maximum of nine α -variants. Under the six loading directions applied in our MD simulations, we observed seven of them $(\alpha 1 \sim \alpha 7)$. Of these, the basal planes come from five $\{01\bar{1}1\}_{\omega}$ planes and two $\{11\bar{2}0\}_{\omega}$ planes of the parent ω -phase. As shown in Fig. 6, $\alpha 1$ and $\alpha 2$ form the $\{11\bar{2}2\}_{\alpha}$ twin; $\alpha 1$ and $\alpha 3$ form the $\{10\bar{1}2\}_{\alpha}$ twin; $\alpha 4$, $\alpha 5$, and $\alpha 6$ form the threefold $\{10\bar{1}1\}_{\alpha}$ twin; and $\alpha 5$ and $\alpha 7$ form the $\{10\bar{1}1\}_{\alpha}$ twin.

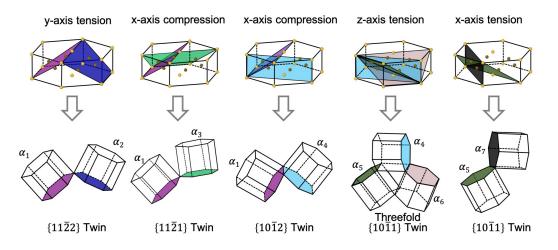


FIG. 6. Schematics showing the formation of seven α -variants ($\alpha 1 \sim \alpha 7$) and five corresponding twins as a result of the $\omega \to \alpha$ martensitic phase transformation. In our MD simulations, two $\{11\bar{2}0\}_{\omega}$ planes (highlighted in light blue and black in the ω unit cells) and five different $\{01\bar{1}1\}_{\omega}$ planes (highlighted in purple, blue, green, pink, and dark green in the ω unit cells) directly transform into basal planes of $\alpha 1 \sim \alpha 7$. The same color scheme as in Fig. 5 is used to highlight the plane correspondence. The arrows represent the $\omega \to \alpha$ martensitic phase transformation.

F. Potential energy evolution

Besides the above crystallographic analysis of the twin formation process, we further examine the evolution of the potential energy for four types of transformation twins. Regions of approxi-

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mately 400 atoms around the transformation twins are traced and their potential energy evolution is shown in Fig. 7. Additionally, the microstructure at the instants of large energy change are included as inset in Fig. 7. In all four cases, the potential energy shows two sharp increases—corresponding to the sequential formation of two α -variants—before reaching the peak. Subsequently, the consumption of the parent ω -phase by the α -variants leads to moderate drops in the potential energy because the α -phase has a lower cohesive energy than the ω -phase in the embedded-atom method potential (ΔE =7 meV/atom). Larger drops in the potential energy are observed for the formation of twin boundaries. Finally, the coherent twin boundaries have a slightly lower potential energy than that in the initial ω -phase.

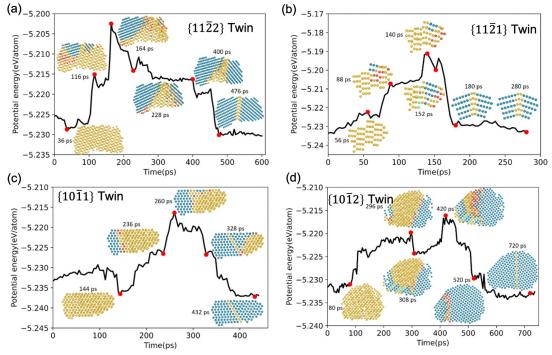


FIG. 7. The evolution of the average potential energy during the formation of four types of transformation twins. The microstructure at the instants of large potential energy change are included as inset.

During this process, there are two competing factors that cause the potential energy to initially increase and then decrease. The first one is a bulk contribution from the energy difference between the α - and ω -phases (ΔE =7 meV/atom in the embedded-atom method potential). The second one is an interfacial contribution from the excess energy of the amorphous and β atoms in the α - ω interfaces. Notably, the interfacial contribution dominates at the beginning and thus the potential energy keeps increasing, because the β -phase has an excess energy ($\Delta E_{hcp-bcc}$ =74 meV/atom)

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one order of magnitude higher than that of the ω -phase ($\Delta E_{hcp-\omega}$ =7 meV/atom). After reaching the peak, the bulk contribution dominates due to the large amount of transformed atoms, leading to a moderate energy drop. The most prominent energy drop comes from the formation of twin boundaries, which replaces the α - ω interfaces and eliminates the interfacial contribution. In particular, the formation of twin boundaries are associated with the abrupt energy drops at 476 ps in Fig. 7a, at 180 ps in Fig. 7b, at 328 ps in Fig. 7c, and at 520 ps in Fig. 7d. In addition, smaller energy drops are identified to correspond to dislocations slip in the ω -phase—at 152 ps in Fig. 7b—and in the α -phase—at 308 ps in Fig. 7d.

IV. DISCUSSIONS

A. The role of initial defects

As discussed in Section IIIB, our MD simulations reveal significant phase transformation-induced plasticity in ω -Ti without brittle fracture under all the loading directions. We note that previous studies mostly reported ω -phase as a brittle phase ^{6,38,39}. This is not in conflict with our work. In fact, the ω -phase studied in those studies was rather stable due to alloying with niobium or other elements, which does not transform into α -phase upon deformation. In contrast, the plasticity (or ductility) observed in our MD simulations on quenched pure Ti is caused by ω -to- α phase transformation, instead of the ω -phase itself. Furthermore, we note that the extensive phase transformations in quenched pure Ti is not surprising. First, the ω -phase has a slightly lower (by 7 meV/atom) energy than the α -phases; as a comparison, the β -phase is 110 meV/atom higher in energy than the α -phase. Accordingly, the elastic strain energy served by external loading can well activate ω -to- α phase transformations. Second, our Ti structure contains plenty of defects that assist the activation of ω -to- α phase transformation to accommodate the plastic deformation, as discussed next.

It is well known that the rate-limiting step of martensitic phase transformation is the initial nucleation, which usually starts from material defects⁴⁰. Therefore, the high transformation-induced plasticity observed is attributed to the initial defects in the quenched ω -Ti structure that serve as martensite embryos, facilitating the nucleation step of the stress-induced martensitic phase transformation. To confirm the role of initial defects, we simulate the deformation of a pristine single crystal ω -Ti with a similar domain size $(27.6 \times 25.89 \times 22.56 \ nm^3)$ as the quenched ω -Ti structure

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Loading type	[0001] T	[0001] C	[1120] T	[1120] C	[1100] T	[1100] C
0.2 strain	3.2%	50.4%	91.9%	10.1%	15.1%	10.8%
0.3 strain	5.3%	63.1%	91.1%	14.8%	50.9%	18.7%

TABLE II. The percentage of α -phase in the

single-crystal ω -Ti at the strain of 0.2 and 0.3 under various loading directions. "T" and "C" represent tension and compression, respectively.

ture. As shown in Table II, the percentage of the α -martensite in the former is much lower than that in the latter. Specifically, at a strain of 0.2, the pristine single crystal only contains \leq 15% α -phase under four loading directions. In contrast, the quenched Ti contains mostly α -phase under four loading directions and \sim 50% α -phase in the other two loading directions.

B. The mechanism of $\omega \rightarrow \alpha$ phase transformation

Because of the metastable nature of the ω -phase, $\omega \rightarrow \alpha$ phase transformation has rarely been studied, though its reverse process— $\alpha \rightarrow \omega$ phase transformation—has been investigated by both experiments and atomistic simulations^{35,41–49}. Specifically, two orientation relations have been established for $\alpha \rightarrow \omega$ martensitic phase transformation, commonly referred to as Variant I (OR I) and Variant II (OR II) following Usikov and Zilbershtein's notation³⁵:

OR I:
$$(0001)_{\alpha} \parallel (01\bar{1}1)_{\omega}, [11\bar{2}0]_{\alpha} \parallel [\bar{1}011]_{\omega}$$
 (1)

OR II:
$$(0001)_{\alpha} \parallel (11\bar{2}0)_{\omega}, [11\bar{2}0]_{\alpha} \parallel [0001]_{\omega}.$$
 (2)

Usikov and Zilbershtein calculated the orientation relation of $\alpha \rightarrow \omega$ phase transformation using the well-known correspondence matrices of $\alpha \rightarrow \beta$ and $\beta \rightarrow \omega$ phase transformations and they obtained two crystallographically nonequivalent orientation relations. Their calculation involves an intermediate β -phase and is regarded as an indirect transformation pathway, while direct ones—TAO-1⁴⁶ and Silcock⁴¹ pathways—have also been developed for $\alpha \rightarrow \omega$ phase transformation. It should be noted that the TAO-1 pathway conforms to OR I, while the Silcock pathway conforms to OR II. The TAO-1 pathway was found to have an energy barrier approximately a quarter of the Silcock pathway, although both orientation relations were observed experimentally $^{35,41-45,47,49}$.

A careful examination of the $\omega \rightarrow \alpha$ phase transformation in our MD simulations reveals that it also follows either OR I or OR II for $\alpha \rightarrow \omega$ phase transformation. To demonstrate this, two

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groups of atoms are traced in our MD simulations and are shown in Fig. 8. In OR I (Fig. 8a), seven atoms in a corrugated $\{01\bar{1}1\}_{\omega}$ plane are highlighted by different colors: three black atoms from the top B-plane of the A1B₂ structure, one purple atom from the middle A-plane, three pink atoms from the bottom B-plane. After the phase transformation, these seven atoms form the basal plane of α -phase: a regular hexagon around a central atom. In contrast, in OR II (Fig. 8b), seven purple atoms in the same $\{11\bar{2}0\}_{\omega}$ plane—four from the B-plane and three from A-plane—will form the basal plane of α -phase. It should be noted that the $\omega \rightarrow \alpha$ phase transformation following OR I observed in our MD simulations always involves a thin layer of β -phase at the ω - α interface, which can be considered as the signature of OR I.

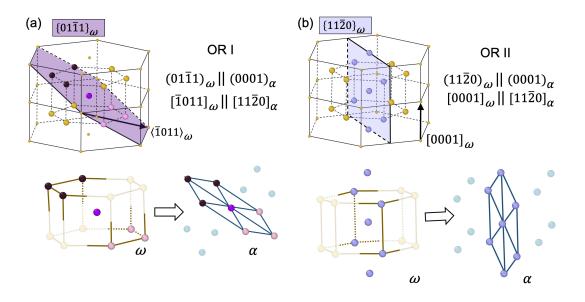


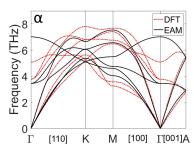
FIG. 8. Two groups of atoms are traced to demonstrate OR I (a) and OR II (b). (a) Top row: one $\{01\bar{1}1\}_{\omega}$ plane spanning over two ω -unit cells is highlighted in purple, in which the atoms traced during the phase transformation have a larger size. Bottom row: seven atoms in the corrugated $\{01\bar{1}1\}_{\omega}$ plane are highlighted by different colors; three black atoms from the top B-plane of the A1B₂ structure, one purple atom from the middle A-plane, three pink atoms from the bottom B-plane. These seven atoms form the basal plane of α -phase under the phase transformation. (b) Top row: one $\{11\bar{2}0\}_{\omega}$ plane spanning over two ω -nit cells is highlighted in light purple, in which the atoms traced during the phase transformation have a larger size. Bottom row: seven purple atoms in a $\{11\bar{2}0\}_{\omega}$ plane form the basal plane of α -phase after the phase transformation.

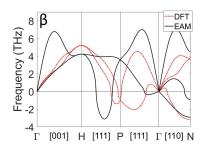
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C. The phonon dispersion relations

It is evident that the martensitic phase transformation between the ω -Ti and α -Ti plays a key role in the formation of transformation twins. To ensure that our MD simulation results reasonably reflect the realistic phase transformation process in Ti, we compare the detailed phonon band structure (i.e., dispersion relations) calculated from lattice dynamics (using the same embedded-atom method potential as that in our MD simulations) with that obtained from density-functional theory calculations³⁴.

Figure 9 shows the phonon dispersion curves for the three Ti phases, α , ω , and β . Obviously, the phonon dispersion curves calculated using the embedded-atom method potential agree reasonably with those from density-functional theory calculations. Notably, the β -Ti has negative phonons around the N-point and the P-point, corresponding to the dynamic instabilities of the [110] transverse-acoustic phonon branch and $\frac{2}{3}$ [111] longitudinal-acoustic phonon branch, respectively. The former causes the phase transformations from β - to α -Ti, while the latter causes the transformation from β - to ω -Ti. As a result, β -Ti is only stabilized by phonon entropy at high temperatures⁵⁰.





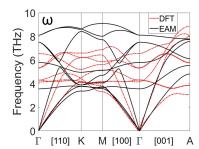


FIG. 9. The comparison between the phonon dispersion curves obtained from our lattice dynamics calculations (EAM) and those obtained from density-functional theory (DFT) calculations³⁴ for the three Ti phases, α , ω , and β .

For ω -Ti, the density-functional theory result shows stiffer phonon modes along the [001] branch than the basal plane directions ([100]) due to the c/a ratio of 0.613. In contrast, the phonon dispersion from embedded-atom method potential displays stiffer phonon modes for basal plane directions than those in the [001] branch, which is attributed to the larger c/a ratio of 0.637 in the embedded-atom method potential. This deviation would predict different elastic response of the ω -phase, but should not adversely affect the twin formation process. This is further confirmed

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by that the same twin formation process is predicted by the modified embedded-atom method potential that successfully captures the stiffer [001] phonon³⁴, as shown in Fig. 4f.

V. CONCLUSIONS

In summary, our MD simulations demonstrated that ω -Ti can undergo significant plastic deformation owing to stress-induced $\omega \to \alpha$ martensitic phase transformation, assisted by the initial defects in the quenched ω -Ti structure. Moreover, we discovered that the stress-induced $\omega \to \alpha$ martensitic phase transformation can lead to the formation of four types of transformation twins in hcp Ti, $\{11\bar{2}1\}$, $\{11\bar{2}2\}$, $\{10\bar{1}2\}$, and $\{10\bar{1}1\}$ twins. We found that the type of the twins—which is defined by the misorientation angle between the two α -variants—is determined by the orientation relation of the $\omega \to \alpha$ martensitic phase transformation. Specifically, two separate OR I can form a $\{11\bar{2}1\}$ or a $\{11\bar{2}2\}$ twin, one OR I and one OR II can form a $\{10\bar{1}2\}$ or a $\{10\bar{1}1\}$ twin, and two separate OR I plus one OR II can form a threefold $\{10\bar{1}1\}$ twin. Our findings expand the type of transformation twins in hcp Ti from only $\{10\bar{1}1\}$ twin^{11,19} to four different types and unveil the essential role of the metastable ω -phase in the formation of transformation twins. This work sheds light on the deformation process and mechanical properties of Ti alloys containing the ω -phase.

AUTHORS' CONTRIBUTIONS

A.Z. and J.O. contributed equally to this work. L.C. designed and directed the project. All authors discussed the results and contributed to the writing of the manuscript.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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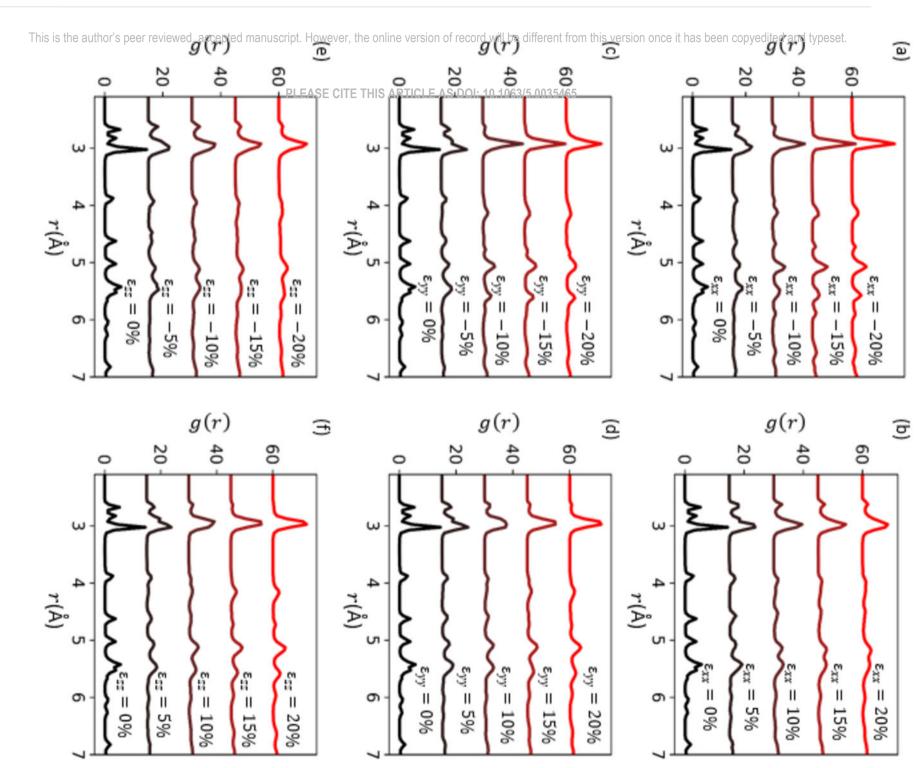


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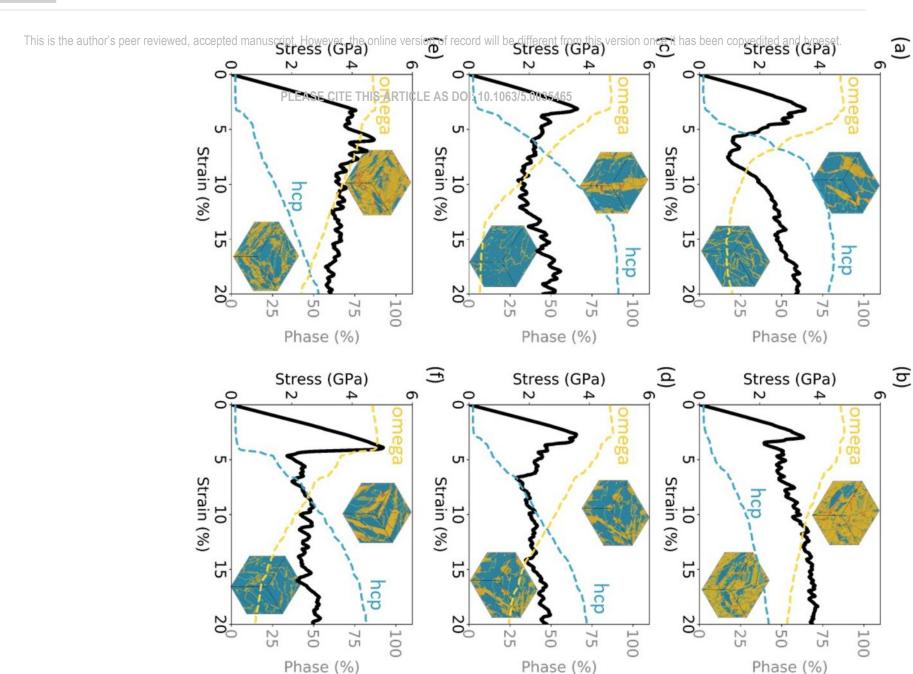
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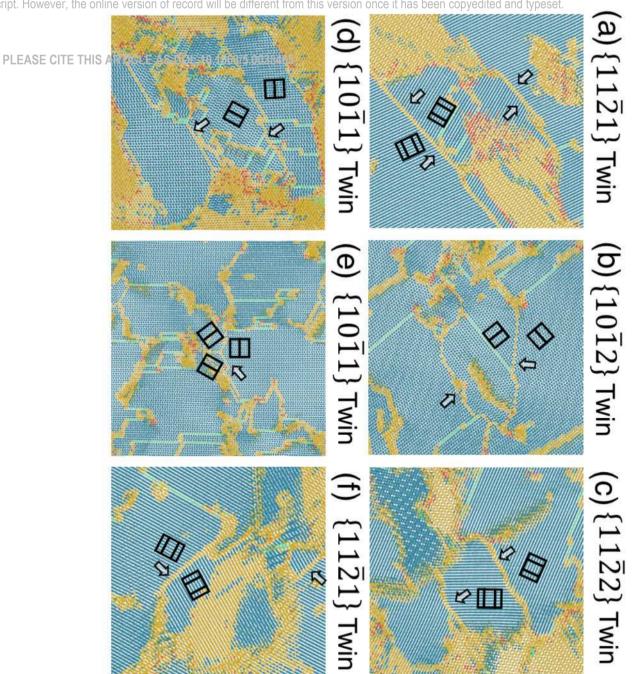
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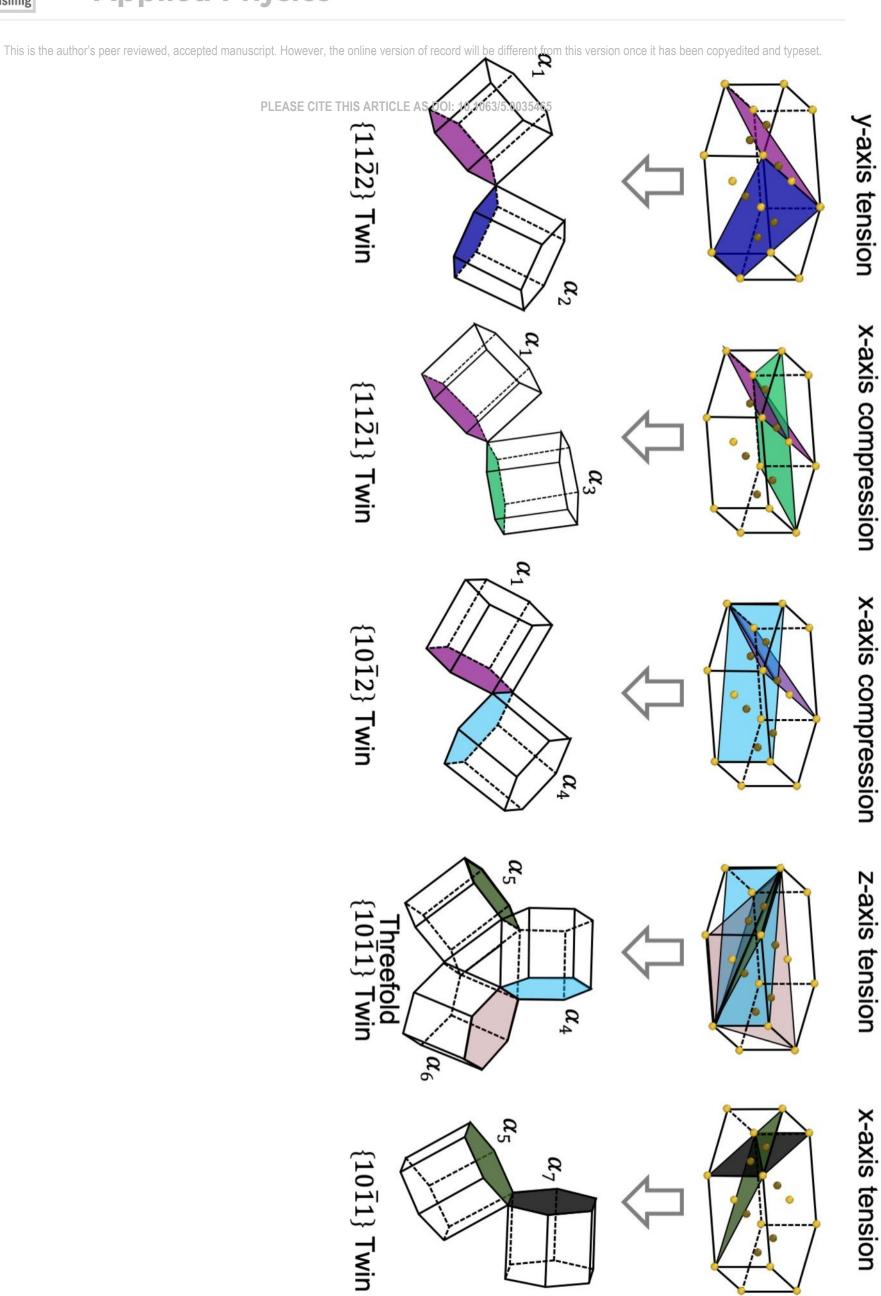


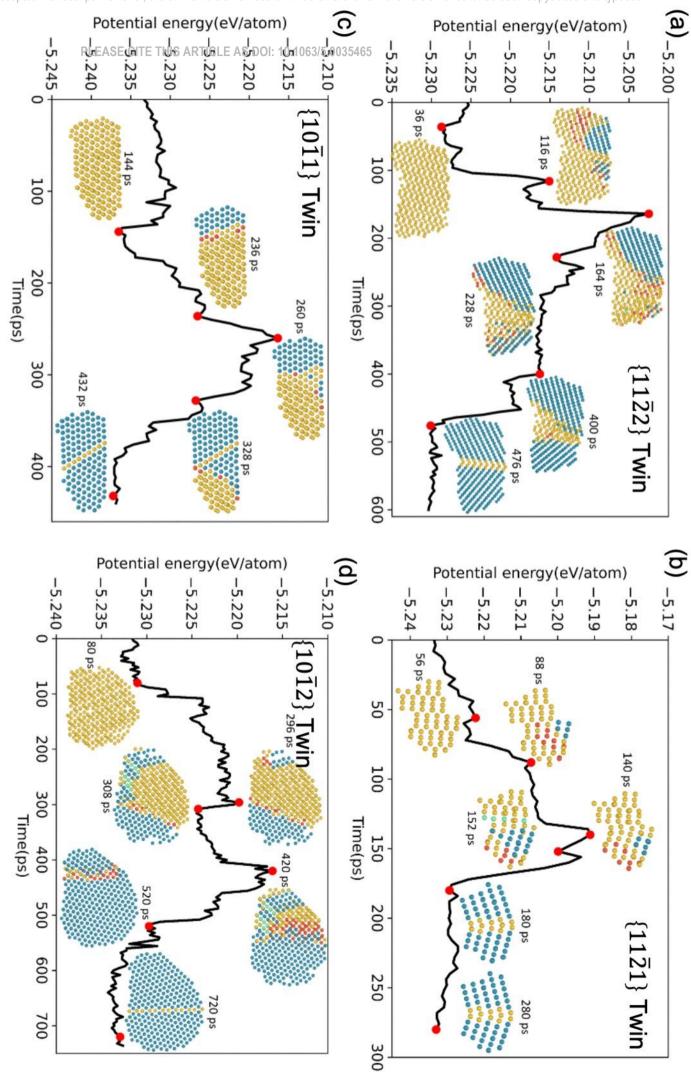


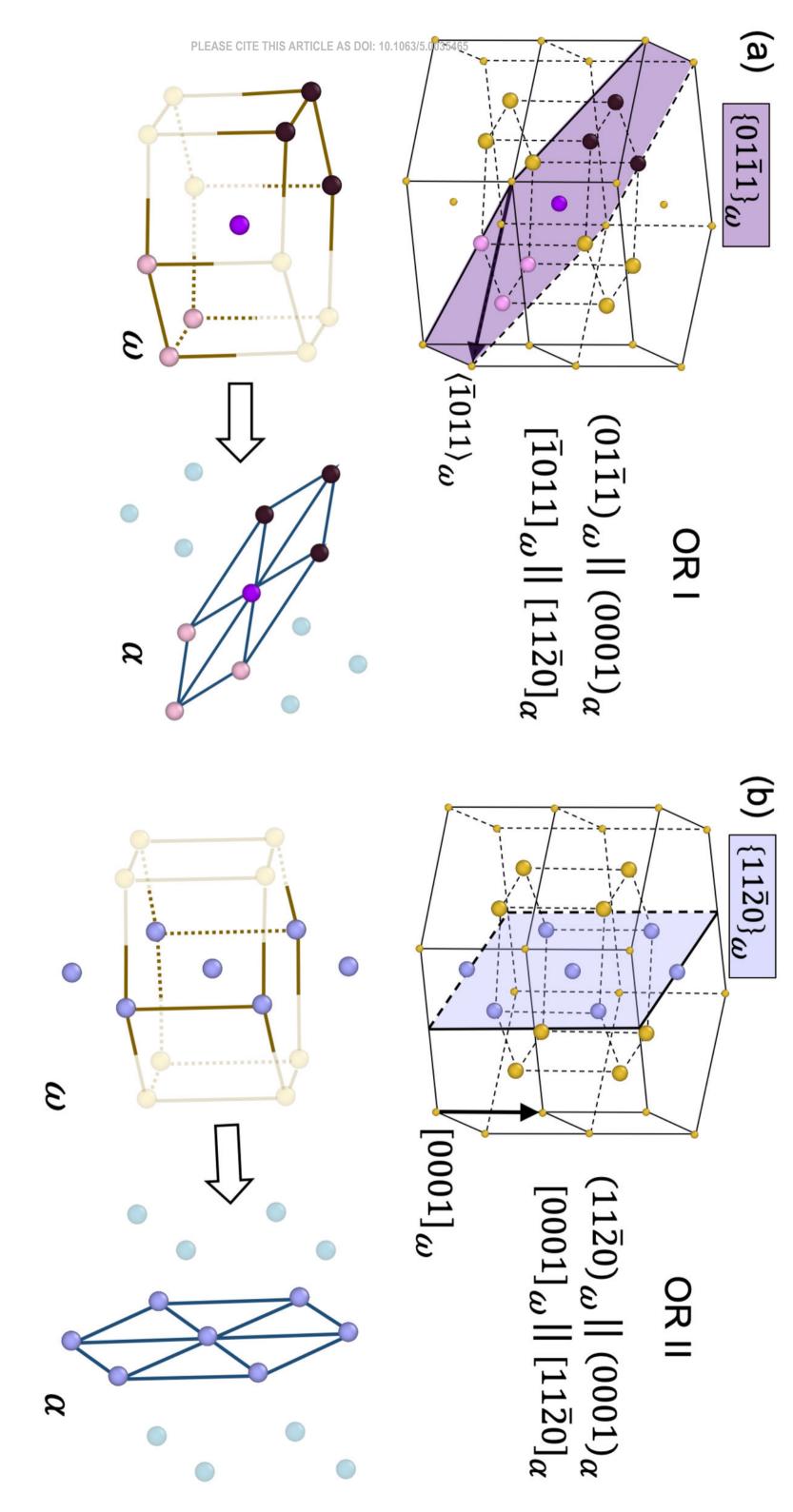
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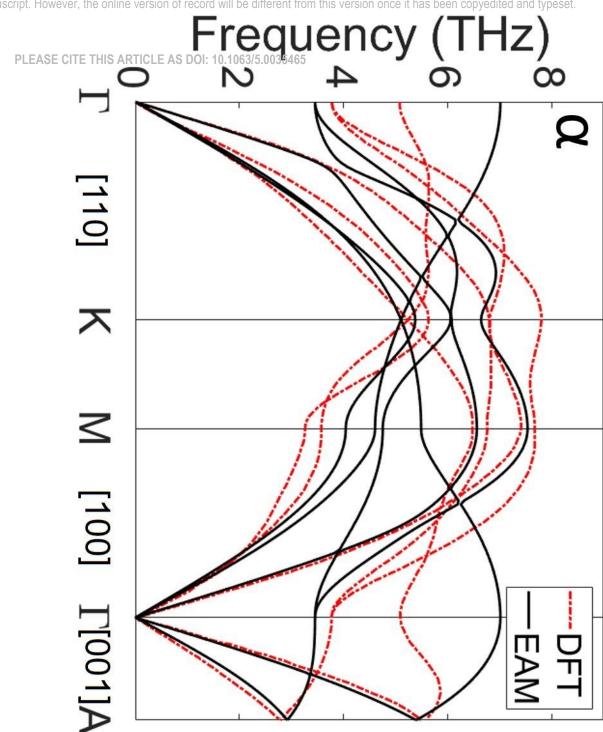
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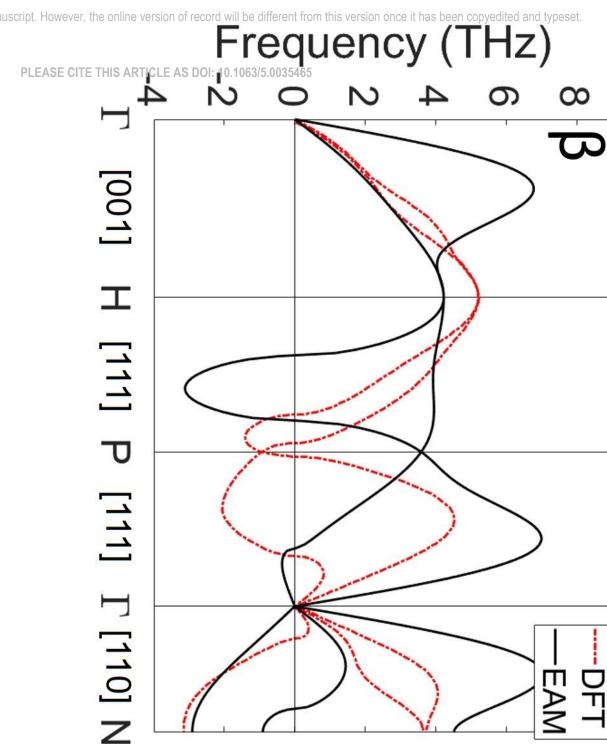














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