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ORIGINAL REPORT



Atomistic mechanism of nucleation and growth of a face-centered orthogonal phase in small-sized single-crystalline Mo

Yan Lu^a, Shiduo Sun^a, Yongpan Zeng^b, Qingsong Deng^a, Yanhui Chen^a, Yangzhong Li^c, Xiaoyan Li^b, Lihua Wang^a and Xiaodong Han^a

^aBeijing Key Lab and Institute of Microstructure and Properties of Advanced Materials, Beijing University of Technology, Beijing, People's Republic of China; ^bCenter of Advanced Mechanics and Materials, Applied Mechanics Laboratory, Department of Engineering Mechanics, Tsinghua University, Beijing, People's Republic of China; ^cHigh Performance Computing Department, National Supercomputing Center in Shenzhen, Shenzhen, People's Republic of China

ABSTRACT

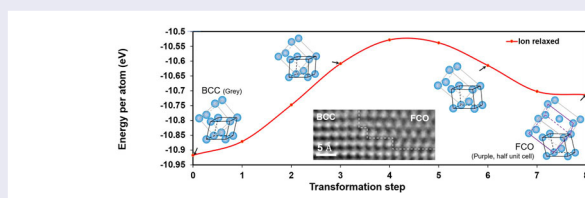
Phase transformation is an important deformation and blunting mechanism at the crack tip of body-centered cubic (BCC) metals. The BCC-to-face-centered orthogonal (FCO) transformation was only predicted by *ab initio* calculations. In this paper, the deformation behavior of the nano-sized single-crystalline Mo is *in situ* investigated in a high-resolution transmission electron microscope at room temperature. We uncover the strain-induced BCC-to-FCO phase transformation. The FCO Mo grows in a layer-by-layer fashion. It is a metastable phase after stress releasing, as confirmed by our *ab initio* calculation. The BCC-to-FCO phase transformation is realized via lattice shearing and shuffling.

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In situ TEM; body-centered cubic metals; phase transformation; deformation mechanism



IMPACT STATEMENT

This paper provides direct *in situ* atomic-scale evidence of BCC–FCO phase transformation, which has never reported on the experimental level.

Introduction

Body-centered cubic (BCC) structured metals are normally with high strength and excellent chemical durability, which can be potentially used in mechanical engineering materials [1–3], nano-electronics devices, semiconductor industry [4–6] and high temperature environments [7,8]. In practical application, the metals are always under stress or in strain environments. Understanding the mechanisms of the microstructural evolution of stressed BCC metals is an essential step for improving their mechanical properties and practical applications in devices. Therefore, the deformation mechanisms of BCC metals have been extensively investigated for several decades, especially of metals with small

sizes. It has been well established that dislocation activities are the most common deformation mechanisms at room temperature in the stage of homogeneous plastic deformation, as confirmed by many experiments on BCC metals, such as α -iron, tungsten, molybdenum, niobium [9–14]. After crack nucleation, the high stress concentrated at the crack tip can active phase transformation, leading to crack blunting, which plays an important role in the toughness performance of BCC metals. Over several decades, phase transformation has been extensively investigated. Since the proposal of the Bain phase transformation path 95 years ago [15], several phase transformation paths have been predicted for BCC metals by previous studies. For example, the

CONTACT Lihua Wang ✉ wlh@bjut.edu.cn Beijing Key Lab and Institute of Microstructure and Properties of Advanced Materials, Beijing University of Technology, Beijing 100124, People's Republic of China; Xiaodong Han ✉ xdhan@bjut.edu.cn Beijing Key Lab and Institute of Microstructure and Properties of Advanced Materials, Beijing University of Technology, Beijing 100124, People's Republic of China

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BCC-to-face-centered cubic (FCC) transformation has been predicted by molecular dynamics (MD) simulations [16–18] in α -Fe and Ta [19] and has been experimentally observed in a transmission electron microscope (TEM) [20,21] in sub-microsized Mo in front of the crack tip. The BCC-to-hexagonal close-packed (HCP) transformation was observed in shock-compressed bulk Mo [22] and the crack area in α -Fe by MD simulation [23]. The BCC-to-face-centered tetragonal (FCT) and BCC-to-face-centered orthogonal (FCO) transformations were predicted by *ab initio* calculations in Mo and Nb [24], which showed that during BCC-to-FCO path, the lattice parameters of Mo changed dramatically and there was an energy saddle point. The finding indicates that FCO-structured Mo should be a stable phase that can be experimentally observed during straining. However, so far, no direct evidence that the BCC–FCO transformation indeed exists has been secured.

To secure experimental evidence and reveal the underlying mechanisms, the deformation behaviors at the crack tip of nano-sized single-crystalline Mo was *in situ* investigated with a homemade tensile device [25,26] in a high-resolution TEM (HRTEM). As the size of Mo decreases to the nano scale, it will suffer higher stress [27–30], increasing the possibility of triggering the BCC–FCO transformation. In the current study, we experimentally demonstrate that the BCC–FCO transformation can indeed occur at room temperature. *In situ* atomic-scale observation shows that the BCC–FCO transformation was achieved via lattice shearing and shuffling, corroborated by the first-principle calculations.

Experiments and calculations

The TEM samples were prepared using an FEI dual beam of the focused ion beam (FIB). First, the [001] zone axis of bulk single-crystalline Mo was dug out using electron back-scattered diffraction. Then, the thin slices normal to [001] zone axis were lifted out and transferred to a homemade uniaxial tension device in FIB. The sample was thinned below 80 nm in thickness and finally polished under a low voltage of 2 kV. The homemade tensile device is mainly composed of two thermal-activated bimetallic strips. These two bimetallic strips are parallel-fixed on a TEM copper-ring grid using epoxy resin. The metals with high thermal expansion coefficients are placed inside and low outside. Using a Gatan double-tilt heating holder, two strips bend outside while the temperature slightly increases, leading to the tension of sample. The temperature applied was below 50°C, which was only 0.17 T_m of Mo (T_m is the melting point of Mo). Thus, the heating effect on the sample can be neglected. *In situ* experiments were conducted in an FEI Titan ETEM at

an accelerating voltage of 300 kV. The energy-step curves were figured out with *ab initio* calculations on Vienna *Ab Initio* Simulation Package (VASP) using the PAW pseudopotential and the GGA exchange–correlation functional [31]. The calculations consider 14 valence electrons for Mo ($4p^6 4d^5 5s^1$). The convergence criterion for electron relaxation is 10^{-4} eV among consecutive steps. For ionic relaxation, the convergence criterion is that all forces decrease to below 0.001 eV/Å. The precession setting ‘PREC = Accurate’ is used. The energy cutoff is set to be 243 eV for all structures.

Results and discussion

Figure 1 shows a series of *in situ* HRTEM images captured in front of a crack tip in single-crystalline Mo, viewing along [001] direction. The relative times are marked at the top right. Figure 1(a) provides a typical HRTEM image captured before the crack propagates, where high-density dislocations can be observed. The lattices exhibit a square shape, and the tensile direction is indicated by a white double-head arrow. Dislocation 1 is marked by a green arrow, serving as the reference to trace the same position, and dislocation 2 is labeled by a white-colored T to indicate the position of the upcoming crack tip. As strain increases, the crack propagates and a small grain with 2 nm width and 4 nm length is generated, as shown in Figure 1(b). The lattices of the newly nucleated grain exhibiting rhombus-shape are obviously different from the BCC [001] zone axis and are semi-surrounded by square-shaped [001] lattices of BCC Mo. Careful analysis reveals that this newly nucleated grain is actually in an FCO phase (see more details below). The phase boundary is labeled by a white dashed line. As shown in Figure 1(c)–(e), the size of the new grain increases, and the phase boundary changes during loading, ultimately leading to the new grain growing up to 3 nm in width and 4 nm in length. With extensive loading, as shown in Figure 1(e)–(f), the crack passes through the right side of the new grain and propagates far away. Interestingly, Figure 1(f) indicates that even with no external force acting on, the new grain remains stable, implying the new phase is a stable structure at room temperature. In Figure 1(a), although it can be detected a high density of dislocations in front of the crack tip, the region that witnessed BCC–FCO transformation is defect-free. This defect-free region can sustain high stress with further loading. Additionally, the strain rate (from Figure S1a, b) is high while the new phase generates. The crack propagates forwards by about 5 nm within 2.8 s. Based on this, it is estimated the high stress and strain rate at the crack tip facilitates with phase transformation, which is in compliance with previous studies [23]. At a relative

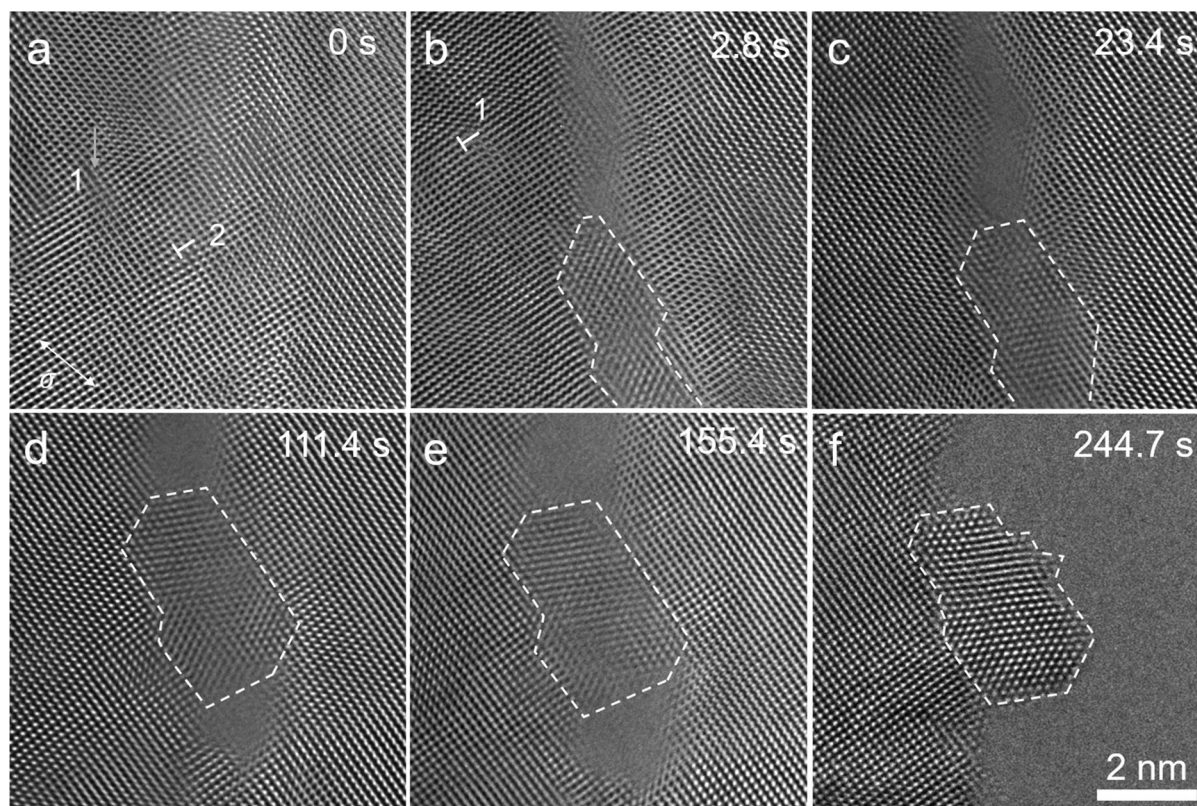


Figure 1. A series of HRTEM images along the BCC [001] zone axis showing the process of phase transformation at a crack tip. (a) Before phase transformation, the lattices exhibit a square shape, consistent with the BCC structure viewing along the [001] zone axis. The white double-headed arrow indicates the tensile direction; two dislocations are marked. (b) Crack propagates, and a new grain nucleates. (c–e) The new grain grows. (f) The new grain is stable after fracture.

low strain rate, dislocation activities could be frequently observed in our experiments.

To determine the crystalline structure of the new lattice, the inter-planar spacing and inter-planar angles were carefully measured during and after the loading process, as shown in Figure 2(a)–(d). In the new grain, three edge-on planes are indicated by blue, yellow and red lines, respectively (Figure 2(a,c)). The intersection angles between them are 61.5° , 61.5° , and 57° , respectively. Additionally, as shown in Figure 2(b,d), the measured spacing of the two neighboring dots on each edge-on plane is $2.7 \text{ \AA}$ (orange), $2.7 \text{ \AA}$ (green), and $2.6 \text{ \AA}$ (red), respectively. The inter-planar angles and dots spacing cannot be calibrated by BCC Mo. According to previous studies, several possible structures of Mo exist, including FCC [20,21,32], HCP [17,23], tetragonal, and orthorhombic structures [24]. Among these structures, it is impossible to calibrate the lattice constants of FCC Mo by using the inter-planar angles and dots spacing of the new grain (see HRTEM simulation images in Fig. S2), and the FCC Mo is with a higher energy barrier in the present shearing path (see energy curve in Fig. S3). These parameters are similar to HCP Mo $\{1\bar{1}00\}$ and $\{22\bar{1}0\}$ planes viewing along the $[0001]$ zone axis ($a = 2.767 \text{ \AA}$,

$c/a = 1.768$) [33], despite the slight variations of inter-planar angles and dot spacing. According to previous *ab initio* calculations [24], the orthorhombic path has lower energy than tetragonal, so the FCO structure is another possibility. Based on our *ab initio* calculations, the FCO structure has a lower energy minimum, while the HCP structure is at a very higher energetic and unstable state, indicating that BCC–HCP phase transformation cannot occur in the present condition (see more details below and Supplementary Fig. S4). Therefore, the new phase should be an FCO structure. According to the measured inter-planar angles and dot spacing, the lattice constants of such FCO Mo are $a = 3.346 \text{ \AA}$, $b = 4.714 \text{ \AA}$, and $c = 3.953 \text{ \AA}$, and the observed zone axis is FCO $[10\bar{1}]$. Additionally, HRTEM simulations of BCC, FCC, HCP and FCO Mo along several low-indexed zone axes were conducted, as shown in Fig. S2. By comparing these simulated images with the experimental results, it is further convincing that the experimental result doesn't match either BCC, FCC or HCP structured Mo while remaining consistently well matched with the FCO-structured Mo viewing along $[10\bar{1}]$ zone axis (as the HRTEM image shown in Figure 2(c)). Figure 2(e) provides the fast Fourier transformed (FFT) image of Figure 2(c), in which

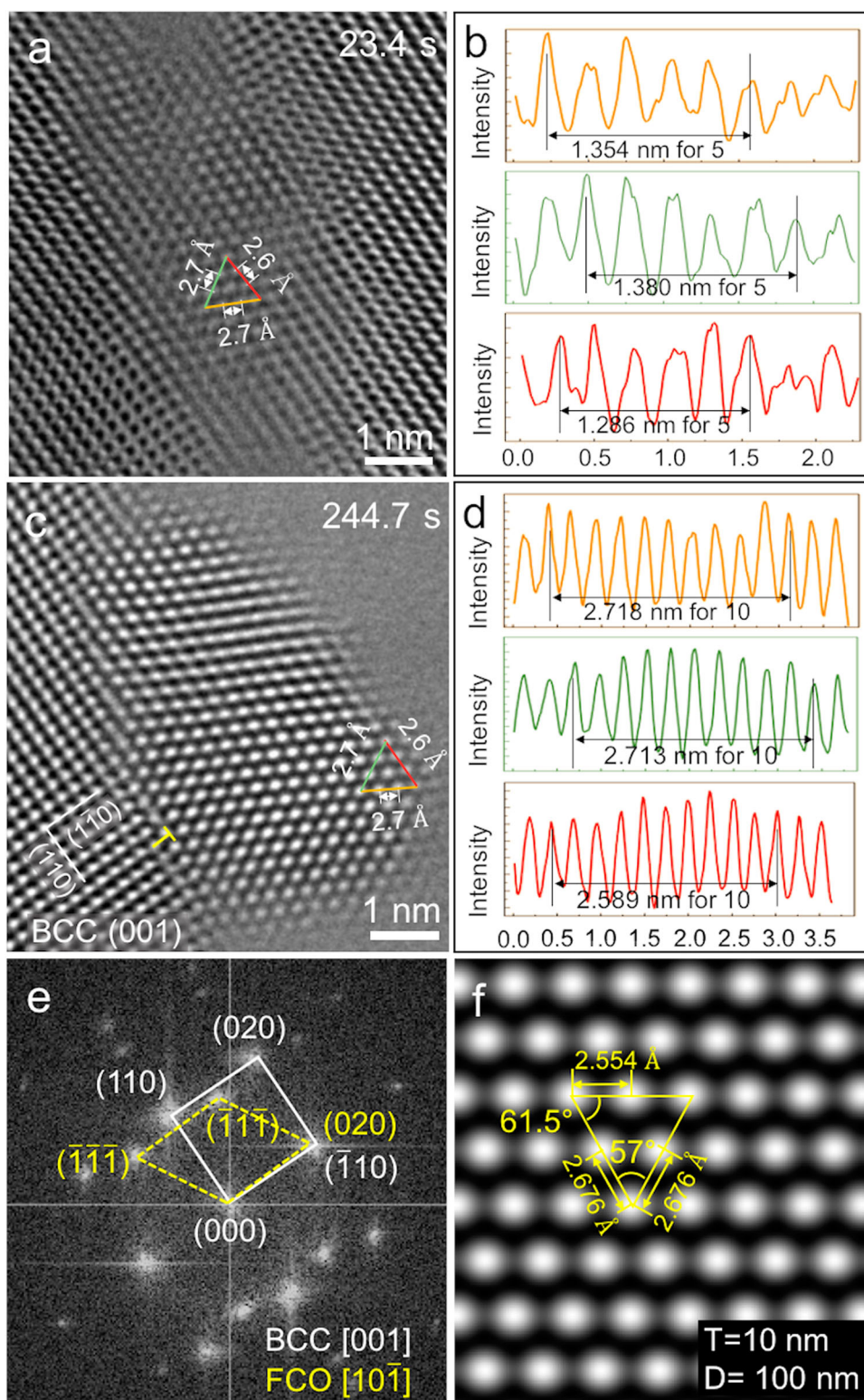


Figure 2. Lattice measurement confirms the BCC-FCO transformation. (a, b) During the new grain growth, the projecting spacing between the two neighboring dots is averagely measured. (c, d) After transformation, the projecting spacing is also averagely measured, which is the same as (a). (e) The corresponding FFT pattern of (c). The spots indexed by white and yellow lines correspond to BCC and the final FCO lattice, respectively. (f) The simulated HRTEM image of the final FCO Mo in the $[10\bar{1}]$ zone axis.

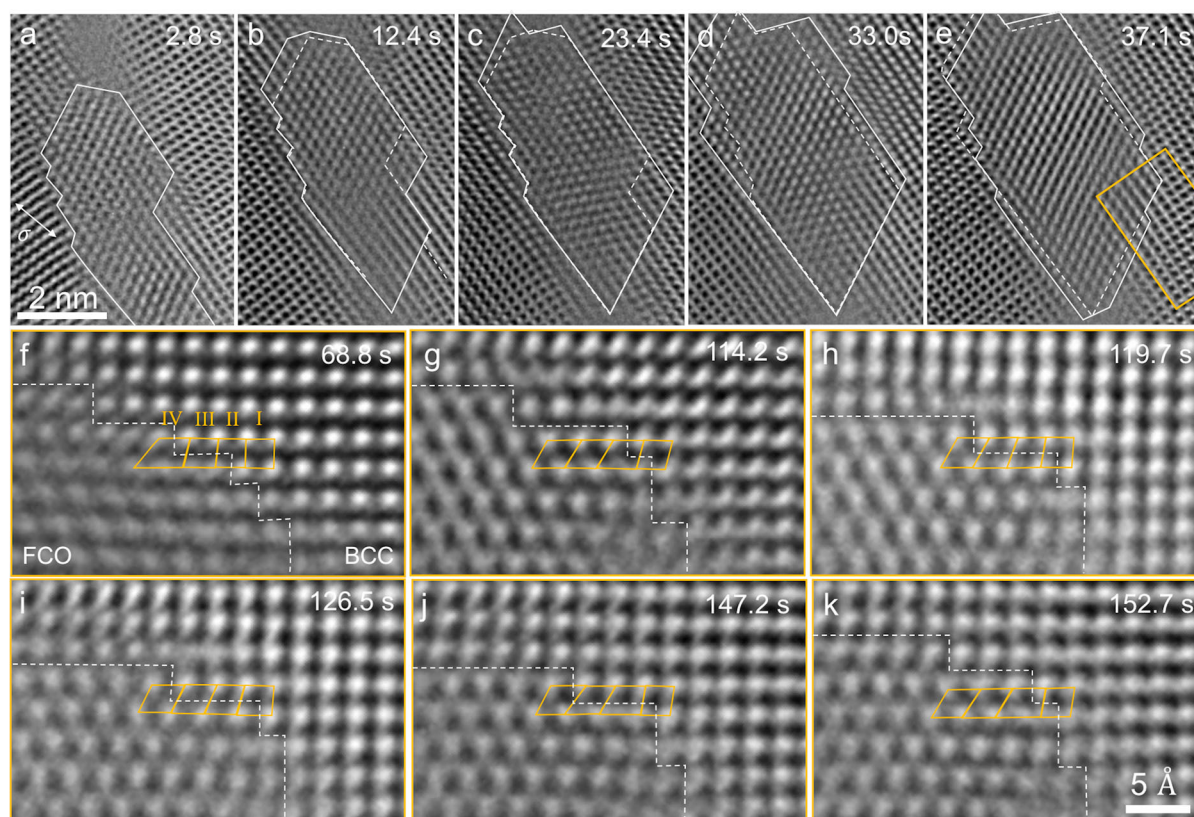


Figure 3. Details of the FCO grain growth. (a–e) The solid lines indicate the present boundary and the dashed lines the previous. (a) The FCO grain is slim. Several steps are observed on the lateral boundaries. (b, c) It expands lengthwise. (d) It grows crosswise. (e) Some lattices at the interface transfer back to BCC lattice. (f–k) The amplified yellow-framed area in (e). The interface is noted by white dashed lines. (f) Four lattices, I–IV, are indicated by four yellow frames. Lattice I is in the BCC structure; lattices II–IV deform. (g) Lattice I becomes diagonal; lattices II–IV further deform. (h–j) The interface reverses back and remains steady. (k) The interface migrates toward the BCC side.

two sets of Bragg diffraction spectrum can be detected, marked by white (BCC lattice) and yellow (final FCO lattice) lines. The simulated HRTEM image of the final FCO Mo along $[10\bar{1}]$ zone axis shown in Figure 2(f) is same as the experimental image.

Figure 3(a)–(e) present the detailed process of the FCO phase growth. The boundary of the FCO grain is indicated by white lines. The solid lines represent the current boundary and the dashed lines previous image. Comparing the dashed and solid lines in the same image allows us to conveniently track the FCO grain growth. In Figure 3(a), the FCO phase is slim, and the lateral interfaces are generally BCC (110) planes despite some steps. As stress increases, in Figure 3(b,c), the FCO phase expands lengthwise, and its width remains. When the right step is filled with fresh FCO lattice, the width begins increasing. In Figure 3(d), comparing the dashed and solid boundaries, the FCO phase mainly grows crosswise and new steps on the lateral boundary are generated. In the following landscapes, same as the above trait, the BCC lattice always transfers into the FCO structure lengthwise

prior to crosswise (Figure 3(a)–(d)). The new FCO lattice expands crosswise layer by layer, leading to width increasing. Moreover, some newly formed FCO lattices are unstable and transfer back to the BCC lattice as shown in Figure 3(e). As shown in Figure 3(a)–(e), the new FCO phase always extends lengthwise prior to crosswise. Considering the crack mode in the current study, the applied stress resolves much higher along lengthwise direction than the crosswise direction. Therefore, the shear stress gradient in the lengthwise direction is much lower than that in the crosswise direction, indicating that the stress decreasing rate in the lengthwise direction is much slower than that in the crosswise direction. Such stress distribution facilitates the new phase growing in a lengthwise direction.

Concerning the atomic-scale mechanisms of BCC–FCO transformation, Figure 3(f)–(k) display a sequence of HRTEM images showing the FCO phase boundary migration process. The BCC and non-BCC interfaces are marked by white dashed lines. The lattices above the white dashed lines are in the BCC structure while below

in the FCO structure. In Figure 3(f), lattice I is a perfect square, exhibiting BCC feature; lattices II to IV exhibit irregular quadrangles. As strain increases, in Figure 3(g), the square lattice I becomes diagonal. Meanwhile, lattices II–IV also change their inner angles. In Figure 3(g)–(h), the upper parts of lattices II and III shear back to BCC lattice (the structure at interface sometimes is reversible). This phenomenon of reversibility has resulted from the inhomogeneous and unstable stress near the interface of the BCC and FCO phase. Due to the mismatch between the BCC and FCO lattice and the change in the stress field of the crack tip during loading, the stress distributed on the interface is inhomogeneous and unstable, which leads to several atoms around the BCC–FCO interface becoming reversible in some cases. In Figure 3(h)–(j), the interface remains steady, but the lower parts of lattices I–IV gradually shear into the FCO structure. With continuous straining, in Figure 3(k), the interface migrates toward the BCC side, and lattices III and IV shear into the FCO structure. At the crack tip, this shearing process can be frequently observed during the BCC–FCO transformation (see another example in Supplementary Fig. S5). After fracture, the sample is free of applied stress, the local inhomogeneous stress is relaxed to some extent, and no reversible atoms between the BCC and FCO lattice were observed.

Based on *in situ* atomic-scale observation, the energy landscape underlying BCC–FCO phase transformation was evaluated using *ab initio* calculations. The BCC structure was constructed as the initial state (Step 0 in Figure 4(a)), and the final FCO structure as the final state (Step 8 in Figure 4(a)). The red curve indicates the ion relaxation of this system, and the blue curve refers to the ion and volume relaxation. In the current study, the BCC and FCO phases have an epitaxial relationship in two BCC $\langle 110 \rangle$ directions; the large lattice misfit strain from the BCC matrix will impede the FCO phase from being fully relaxed in terms of volume, and the FCO phase will get strained to some extent. For the red curve in Figure 4(a), the basic condition is to keep the volume unchanged. The ion-relaxed curve reflects the volume limitation that is similar to our experimental condition. From this curve, the final FCO structure locates at the valley of the energy curve, indicating the new phase is stable. In order to ensure the stability of the FCO phase, the energy of the FCO phase under conditions with both ion and volume relaxation was also calculated as shown by the blue curve in Figure 4(a). Again, the FCO structure at Step 8 of ion and volume-relaxed curve (locates at the valley of the energy curve) is similar to the ion-relaxed curve (Fig. S6), which confirms that the FCO phase in this study is indeed stable. Figure 4(b)–(e) shows the three- and two-dimensional atomic models corresponding to

the initial BCC structure, two transition structures, and the final FCO structure of Mo. In these figures, the lattices linked by grey lines indicate the original BCC unit cells and variants, while the black shows the lattice transformation just as the yellow frames in Figure 3(f)–(k). During the phase transformation, BCC Mo undergoes not only shearing (lattice angle changes) but also shuffling (atomic bond length changes). As indicated in the two-dimensional atomic model, the shearing and shuffling are consistent with the HRTEM observations.

Although the deformation mechanisms of BCC metals have been extensively investigated for decades, most of the previous studies only reported the dislocation activities, BCC–FCC phase transformation, and deformation twinning [9–14]. However, the BCC–FCO transformation has never been observed in experimental conditions. Here, we provide direct dynamic and atomic-scale evidence.

Previously, several types of phase transformation have been observed in BCC metals under different strained conditions [16–20, 23]. The reason for such variations can be considered intrinsic and extrinsic factors for the phase transformation. The high stress and appropriate loading orientation, which can significantly impact the stress state and determine which transition path or new phase will be triggered, is an important extrinsic factor for phase transformation. In this study, the thickness of samples is less than 20 nm, which can suffer high stress according to the principle of ‘smaller is stronger’ [34–36]. The high stress can supply sufficient energy to overcome the energy barrier for phase transformation, while the loading orientation can determine the transition path and the phase type. For example, previous *ab initio* calculation showed that the loading orientation can significantly impact the phase transition path and the related energy barriers [24]. Additionally, the energy barrier of the new metastable phase is an important intrinsic factor for phase transformation. For the new phase with a high energy barrier, it demands ultra-high stress and it’s difficult to generate phase transformation even under the appropriate loading orientation. According to our *ab initio* calculation, HCP Mo can’t generate in the present shearing path (Fig. S4), and FCC Mo is unstable and with high energy barrier (Fig. S3), which is in compliance with previous *ab initio* calculations [33]. However, the FCO-structured Mo is a stable phase with relatively low energy barrier when applied shear stress is along $\langle 110 \rangle$ direction. This confirms that both the extrinsic and intrinsic factors can significantly impact the phase transition path and the related energy barrier, and may be the reason behind several types of new phases being detected under different strain conditions in BCC metals [16–20, 23]. In the current study, the stress direction is

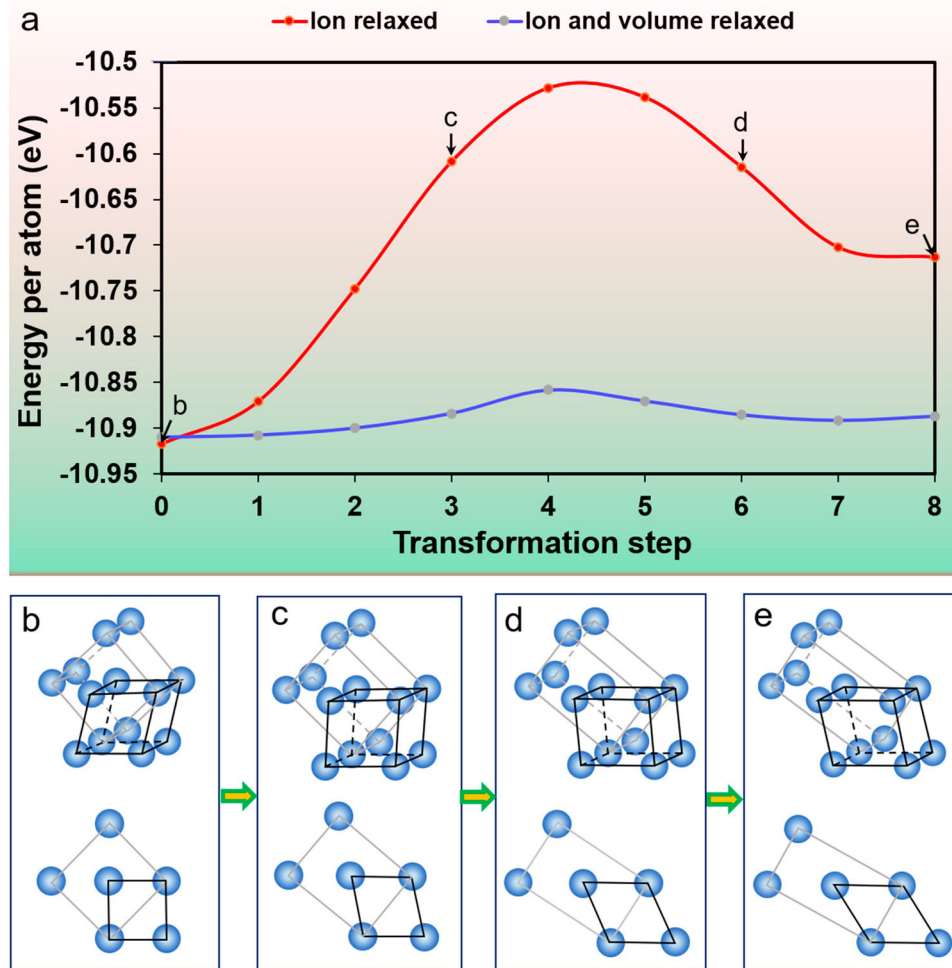


Figure 4. First-principle calculation of BCC-FCO phase transformation. (a) The energy is a function of the transformation step. Step 0 is the BCC structure, step 8 the final FCO structure. The red curve indicates the ion relaxation, the blue ion and volume relaxation. (b–e) The upper figures show the perspective view, the lower showing the front view.

$\sim 15^\circ$ between BCC (110) plane (from Figure 1(a)), and the resolved shear stress on BCC (110) plane is 0.966σ . In conclusion, the appropriate crack orientation and crack mode, as well as the high stress at crack tip and relatively low energy barrier, lead to the BCC-FCO phase transformation. Therefore, it is supposed that the observed BCC-FCO phase transformation is not a special case, and this FCO phase can also generate in a large sample or large grains with appropriate loading orientation combined with high stress.

Such phase transformation will consume a considerable amount of energy, consequently blunting the crack tip, slowing down the crack propagation, and enhancing the toughness of BCC Mo. Our *in situ* atomic-scale experimental results along with previous nanoscale studies and predictive atomistic simulations provide a comprehensive view to understand the deformation mechanism of BCC metals.

Conclusions

With our homemade tensile device, for the first time, the BCC-FCO transformation in nano-sized single-crystalline Mo was *in situ* observed. It is revealed that the newly formed FCO Mo grows in a layer-by-layer fashion. After the stress is released, the FCO phase is stable, corroborated by first-principle calculations. This *in situ* study at atomic resolution sheds light on understanding the deformation mechanisms of BCC metals.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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