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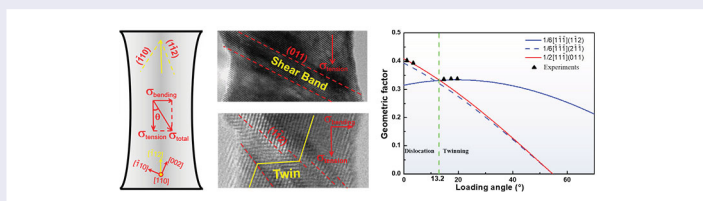
Bending-induced deformation twinning in body-centered cubic tungsten nanowires

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ABSTRACT

The competition between dislocation slip and deformation twinning in body-centered cubic (BCC) nanocrystals can be strongly influenced by the deformation conditions. In this study, we investigate the deformation of [112]-oriented BCC tungsten nanowires under different loading modes. It shows that dislocation plasticity is a predominant deformation mode under uniaxial tension, while deformation twinning prevails when non-uniaxial stress is applied. The interfaces of bending-induced twinning are composed of numerous stepwise {112} twin boundaries. These findings shed light on the deformation mechanism of BCC nanocrystals under complex loading conditions.



IMPACT STATEMENT

In situ nanomechanical testing and quantitative analysis reveal a deformation mechanism transition in tungsten nanowires, from dislocation slip under the uniaxial loading to deformation twinning under the non-uniaxial loading.

ARTICLE HISTORY

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KEYWORDS

Bending; body-centered cubic; twinning; dislocation; tungsten nanowire

1. Introduction

Metallic nanowires (NWs) are of great significance in nanoelectromechanical systems due to their excellent mechanical, electrical and chemical properties [1,2]. A thorough understanding of their structure–property relations, especially mechanical properties, is of critical importance for the wide application of metallic nanostructures. In past decades, numerous studies have been conducted to establish a full deformation map of metallic nanostructures at different length scales, using *in situ* transmission electron microscopy (TEM) techniques and molecular dynamics (MD) simulations [2–5]. These experimental and theoretical studies have revealed a wealth of novel deformation behavior and size-dependent mechanical properties in small volume materials, including dislocation starvation [6], mechanical annealing [7], surface-controlled dislocation nucleation

and yielding [8,9], twinning-dominated deformation [10], and superplastic deformation [11] etc. It is noticed that uniaxial tensile or compressive stresses were usually applied in previous experimental and theoretical studies [8,12,13]. Given that nanocomponents in nanoelectromechanical systems usually experience relatively complex stress conditions, it is necessary to investigate the deformation behavior of metallic nanostructures under non-uniaxial loadings. Recently, bending testing [14–16] was introduced to investigate the mechanical responses of metallic nanostructures under non-uniaxial stress. *In situ* TEM studies and MD simulations did reveal some unprecedented deformation phenomena [15,17], e.g. pseudo-elasticity and wedge-shaped twins in α -Fe nanowires [17] and twin size dependent dislocation activities in nanotwinned Ni nanowires [15]. These bending testing suggest that the deformation mechanisms of

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metallic nanostructures may change with the loading mode and stress condition; therefore, mechanical testing of metallic nanostructures under non-uniaxial loadings need to be conducted in order to obtain a comprehensive understanding of the deformation behavior.

On the other hand, BCC metallic nanostructures are of great significance in many fields due to their high strength and excellent thermal stability; thus the size-dependent mechanical properties of BCC nanostructures have attracted increasing attentions recently. It has been well-established that the deformation of BCC nanopillars with the diameters of 100–500 nm was usually dominated by dislocation activities at room temperature [18,19]; with the size reduction, twinning-dominated deformation showed up in tungsten (W) nanowires around 20 nm under most loading orientations, including $\langle 100 \rangle$ tension, $\langle 110 \rangle$ compression and $\langle 111 \rangle$ compression [12]. However, an exception was the W nanowires under the uniaxial $\langle 112 \rangle$ tension and compression, showing a dislocation-dominated deformation [12,20] due to the competing nucleation of surface defects under ultrahigh stress. To gain further insights into the deformation mechanism transition in W nanowires under different loading modes, the non-uniaxial bending testing provides a good opportunity to study this question.

In this paper, $\langle 112 \rangle$ -oriented W nanowires were tested under different loading modes using *in situ* nanomechanical testing. Under uniaxial $\langle 112 \rangle$ tension, dislocation activities coupled with a shear band governed the deformation; however, under non-uniaxial loading of combined bending and tension, deformation twinning was activated in the $\langle 112 \rangle$ -oriented W nanowires, which acted as the predominant deformation mode through its nucleation and thickening. Atomistic observation shows that the bending-induced deformation twinning possesses stepwise twin boundaries, which is composed of numerous $\{112\}$ atomic facets. The overall morphology of this stepwise twin boundary may have a projection along $\{011\}$ plane when viewed from $\langle 111 \rangle$ direction, which calls for an attention regarding the twinning analysis in BCC metals conducted other than the $\langle 110 \rangle$ zone axis.

2. Experimental methods

The $[112]$ -oriented W nanowires were created by an *in situ* welding method inside a Cs-corrected TEM (FEI Titan G2 60–300) operating at 300 kV [12]. A PicoFemto TEM-scanning tunneling microscope (STM) platform from Zeptools technology Co. was used for experiments. During experiments, nanotooth on the fresh fracture surfaces of two bulk polycrystalline W rods (Purity:

99.98 wt.%, diameter: 0.010 in.) was welded together inside TEM. *In situ* tension and compression were then conducted at room temperature at a strain rate of $\sim 10^{-3} \text{ s}^{-1}$ by moving the W rod on the pizeo-controller side backward along the nanowire axial direction; while the combined bending and tension testing was carried out by moving the W rod on the pizeo-controller rightward at a constant rate of 0.1 nm s^{-1} . Besides, we also deliberately applied the tensile loading deviating from the nanowire axis to study the effect of loading angle on the deformation mechanism (Figure 4). More details about sample fabrication and tension/compression testing can be found in our previous publication [12].

3. Results

Figure 1 demonstrates the typical deformation behavior of $[112]$ -oriented W nanowires under uniaxial loading, showing the dislocation and shear band dominated plasticity. Before deformation, the nanowire (viewed from the $[\bar{1}\bar{1}1]$ direction) has a perfect structure without evident lattice defect (Figure 1(a)), in contrast to the samples with pre-existed defects and surface contaminations fabricated by the focused ion beam method [7,19]. Upon uniaxial tension, strain accumulation caused the preferential surface nucleation of dislocations, from both the side surface and viewing surface [20]. Given the numerous surface nucleation sites in small volume samples [8,21], dislocations can be emitted from different sites homogeneously [12,20], which accumulate inside the crystal due to the low mobility of dislocation in BCC metals [22]. The massive dislocation activities eventually result in the sudden formation of a shear band (Figure 1(b)). Zoomed-in image in Figure 1(c) shows numerous dislocations in the shear band, suggesting the dislocation-induced shear band formation. We also noticed that some of the dislocations nucleate as dipoles, which should be the surface-emitted half dislocation loops on (011) planes. Considering that the deformation twinning also has a band-like structure and that the symmetrical behavior of deformation twinning in BCC metals can only be observed along the $[110]$ direction, uniaxial tension of $[112]$ -oriented W nanowire was further conducted in the $[110]$ zone axis to exclude the possibility of deformation twinning. Figure 1(d) clearly shows that the deformation of $[112]$ -oriented W nanowire was dominated by the dislocation activities, which formed a deformation band with dense dislocations, consistent with the observation in Figure 1(a-c).

To understand the effect of loading mode on deformation, *in situ* nanomechanical testing of $[112]$ -oriented W nanowires was further carried out under non-uniaxial loading by applying combined stress of bending and

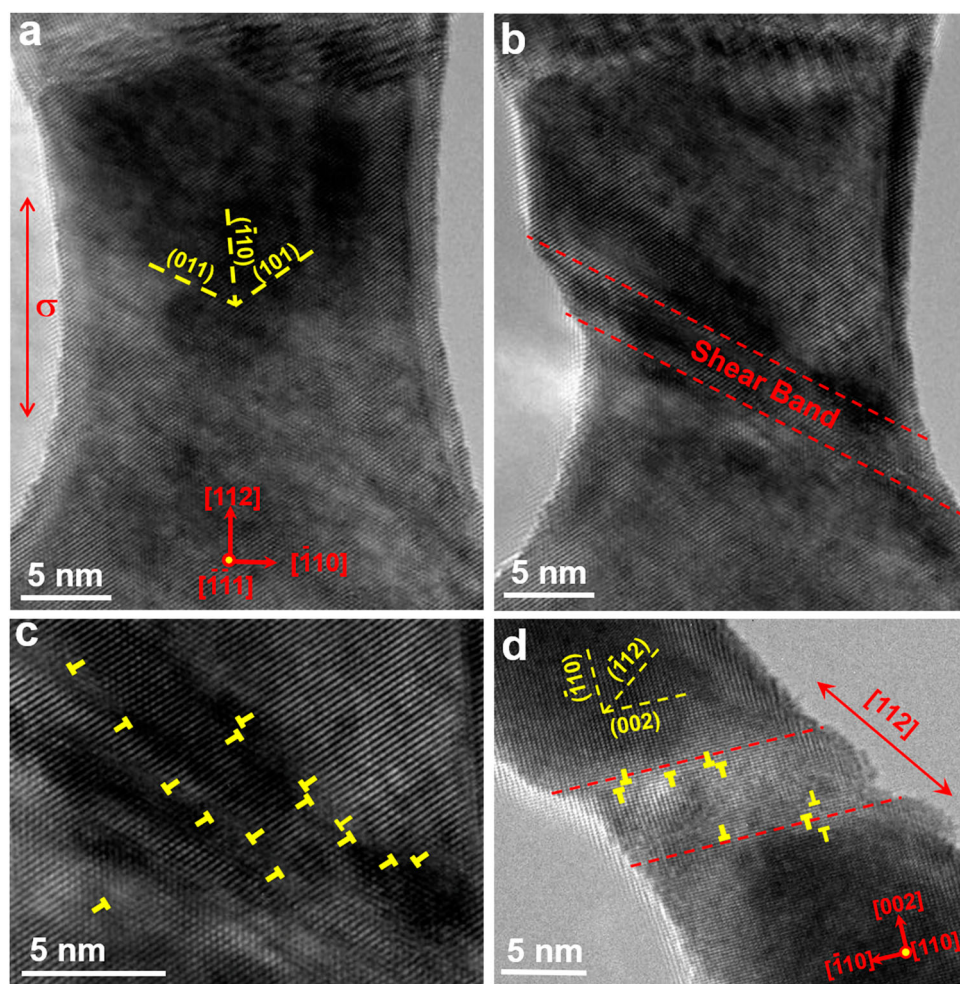


Figure 1. Dislocation-induced shear band plasticity under [112] tension of a W nanowire. (a) The morphology of pristine W nanowire. The tensile direction is along [112] and the viewing direction is along $[\bar{1}\bar{1}1]$. (b) Dislocation-induced Shear band under [112] tension. (c) Zoomed-in image of the shear band. (d) Dislocation-induced shear band in [112]-oriented W nanowire by viewing along the [110] direction.

tension (Figure 2). Figure 2(a) shows the structure of a [112]-oriented W nanowire in $[\bar{1}\bar{1}1]$ zone axis before deformation, without observable lattice defect. *In situ* deformation was initiated by applying a combined loading of bending and tension, resulting in a non-uniaxial stress state. Upon the non-uniaxial loading, no dislocation activity was observed before the yielding of this nanowire, in contrast to the dense dislocation activities under the uniaxial tension. Subsequently, a thick deformation band with an overall interface along the (011) plane formed suddenly with the accumulation of deformation strain, resulting in a kinked deformation morphology of the nanowire, as shown by the pink lines in Figure 2(b). As the strain increased, gradual thickening of the deformation band occurred continuously in the nanowire, which is different from the discrete shear band deformation under uniaxial tension [20]. It is noticed that the kinked structure and the gradual thickening

of this deformation band match well with the deformation twinning induced reorientation (with a kinked nanowire geometry) and the layer-by-layer thickening of deformation twinning in different metallic nanowires [10,23], which suggest that the observed kinked deformation band under non-uniaxial loading of [112]-oriented W nanowire might be a deformation twin. However, the symmetrical behavior of deformation twinning in BCC metals cannot be observed in the $\langle 111 \rangle$ zone axis due to the three-fold lattice symmetry. Given that the loading mode can strongly influence the deformation mechanism of metallic nanowires [15,24], it is necessary to study whether the deformation of [112]-oriented W nanowire under the non-uniaxial loading of combined bending and tension is dominated by deformation twinning, instead of dislocation.

To answer this question, deformation of [112]-oriented W nanowire was further conducted under

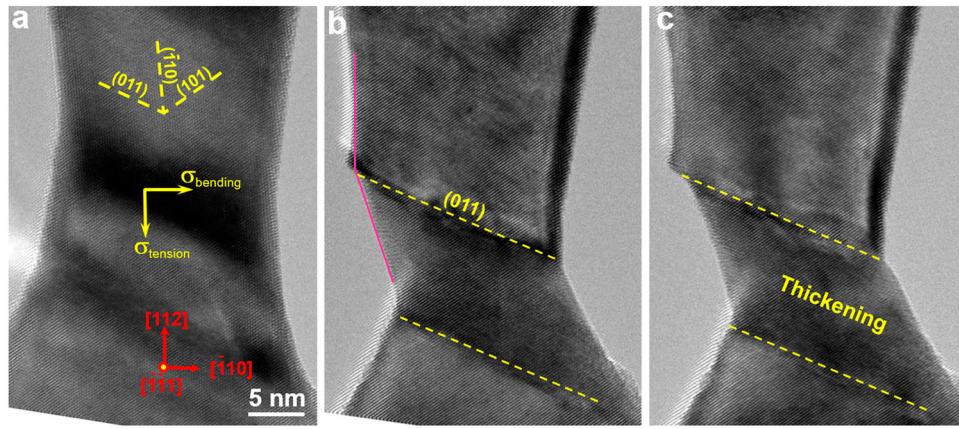


Figure 2. Deformation band in a [112]-oriented W nanowire under the non-uniaxial loading. (a) The morphology of pristine W nanowire, with the viewing direction of $[\bar{1}\bar{1}1]$. (b) Sudden formation of a deformation band with the (011) interfaces under the non-uniaxial loading of combined bending and tension. (c) Layer-by-layer thickening of the deformation band under further loading.

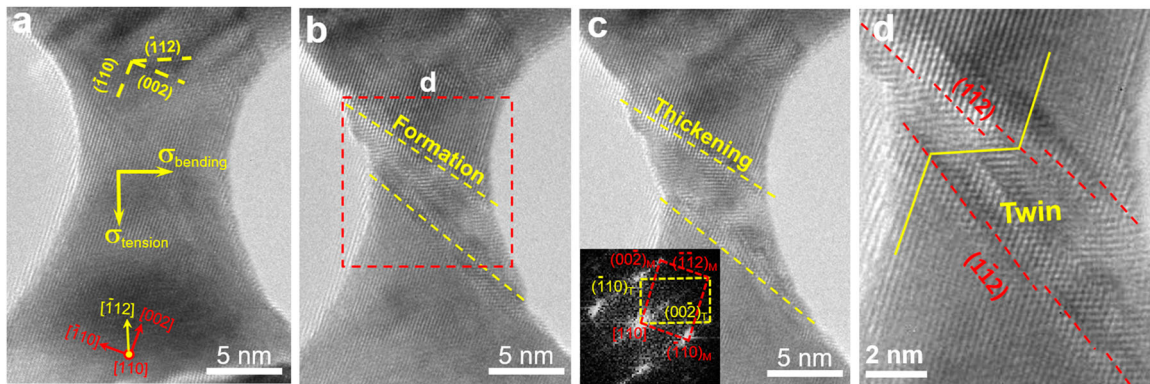


Figure 3. Deformation twinning in a [112]-oriented W nanowire under the non-uniaxial loading. (a-c) Sequential TEM images showing the twinning-dominated deformation in a W nanowire under the non-uniaxial loading of combined bending and tension. The viewing direction is along $[110]$. (d) Zoomed-in image of the deformation twinning. Inset in (c) is the Fast Fourier transform pattern of the deformation twin.

non-uniaxial loading by viewing along the $[110]$ direction, as shown in Figure 3. To exclude unnecessary influence factors, we created a $\langle 112 \rangle$ -W nanowires with similar structure. Before deformation, the nanowire had the same loading geometry as the one presented in Figure 2, but different viewing direction ($[110]$ for Fig. 3). Upon non-uniaxial loading, a deformation band formed in this nanowire (Figure 3(b)), which thickened gradually with the straining (Figure 3(b-c)). The formation of this deformation band also resulted in a kinked nanowire geometry (Figure 3(c)), like the one presented in Figure 2. Close observation indicates that the deformation band is actually a deformation twin (Figure 3(d)), as confirmed by the fast Fourier transformation image in the inset of Figure 3(c). However, this deformation twin possesses stepwise twin boundaries, which is composed of abundant $\{112\}$ atomic facets. Such stepwise twin boundaries also occurred during the shock deformation of BCC Ta [25] and bending deformation of α -Fe nanowires [17],

which was attributed to the separate dissociation of screw dislocations within a slip band [25]. Above results indicate that the kinked deformation band occurred in the $[112]$ -oriented W nanowire under the non-uniaxial loading should be a deformation twinning with stepwise $\{112\}$ twin boundaries, the projection of which presents as an overall interface along (011) planes without twinning symmetry when viewed from $[\bar{1}\bar{1}1]$ direction. This observation calls for an attention when analyzing the deformation structure in BCC metals in $\langle 111 \rangle$ zone axis.

4. Discussion

Above results clearly demonstrate that the loading modes have important influences on the deformation of BCC metallic nanowires. Previous simulations also showed that the non-uniaxial bending can activate some unique deformation behavior in metallic nanowires [17,26], such

as twinning-mediated pseudo-elasticity [17]. In small-volume BCC crystals, the nucleation stresses of dislocation and deformation twinning are comparable [12], such that a dynamic competition between them may occur upon deformation. Given the similar nucleation stresses of dislocation and twinning, their competition should be controlled by the critical shear stresses on the dislocation and twinning systems. Here, the transition from ordinary dislocation plasticity under uniaxial loading to deformation twinning under non-uniaxial loading in $[112]$ -oriented W nanowires can be ascribed to the change of resolved shear stress under the bending loading. Under the uniaxial tension, $[112]$ -oriented W nanowire is in an antitwinning-orientation, such that the nucleation and slip barriers of twinning dislocation on (112) planes are much higher than that of ordinary dislocation [27–29], favoring the dislocation plasticity on (110) planes. Besides, the largest Schmid factors on the dislocation slip and deformation twinning systems for the $[112]$ -oriented W nanowire are 0.41 and 0.39, respectively, further facilitating the dislocation deformation. Under the non-uniaxial loading, the combined bending and tension can be equivalently expressed as a resultant force (defined as σ_{total} in the following) that deviates from the nanowire axis, as schematically shown in Figure 4. Thus, the resolved shear stresses on the $1/6[1\bar{1}\bar{1}](1\bar{1}2)$ twin system (Figure 3) and the $1/2[11\bar{1}](011)$ slip system (Figure 1) of the $[\bar{1}12]$ -oriented nanowires change with the misalignment between the nanowire axis and σ_{total} . The resolved shear stresses on the $[1\bar{1}\bar{1}](1\bar{1}2)$ twin system and the $[11\bar{1}](011)$ slip system can be expressed as:

$$\tau_t = \cos \lambda_t \cos \varphi_t F / A_0, \quad (1)$$

where λ_t is the angle between σ_{total} and the $[1\bar{1}\bar{1}]$ direction, and φ_t is the angle between the normal direction of $(1\bar{1}2)$ plane and the $[\bar{1}12]$ direction; F is the total force, and A_0 is the area of the cross section of the W nanowire.

$$\tau_d = \cos \lambda_d \cos \varphi_d F / A_0, \quad (2)$$

where λ_d is the angle between σ_{total} and $[11\bar{1}]$ direction, and φ_d is the angle between the normal direction of (011) plane and the $[\bar{1}12]$ direction. Here, $\cos \lambda_t \cos \varphi_t$ and $\cos \lambda_d \cos \varphi_d$ are the geometric factors (which is different from the Schmid factors due to that the direction of σ_{total} is not perpendicular to the nanowire cross section) on $1/6[1\bar{1}\bar{1}](1\bar{1}2)$ twin system and $1/2[11\bar{1}](011)$ slip system, respectively. Given the similar nucleation stresses for twinning and dislocation, the deformation on planes with maximum resolved shear stress will be activated upon loading, acting as the predominant plastic deformation mode. For a given σ_{total} , the resolved shear stresses on different slip planes vary with the misalignment between the nanowire axis and σ_{total} . As schematically shown in Figure 4(b), the non-uniaxial loading of combined bending and tension could result in a markedly-increased resolved shear stress on the $1/6[1\bar{1}\bar{1}](1\bar{1}2)$ twin system in $[\bar{1}12]$ -oriented W nanowires if σ_{total} is slightly deviated from the nanowire axis. Figure 4(c) shows the variations of geometric factor for the maximum resolved shear stresses of dislocation and twinning with the misalignment. It is seen that the resolved shear stress for dislocation slip on $1/2[11\bar{1}](011)$ is higher than that of $1/6[1\bar{1}\bar{1}](1\bar{1}2)$ twinning if the misalignment is less than 13.2° , which would favor the dislocation activities. However, when the misalignment is higher than 13.2° , the resolved shear stress for $1/6[1\bar{1}\bar{1}](1\bar{1}2)$ twinning are

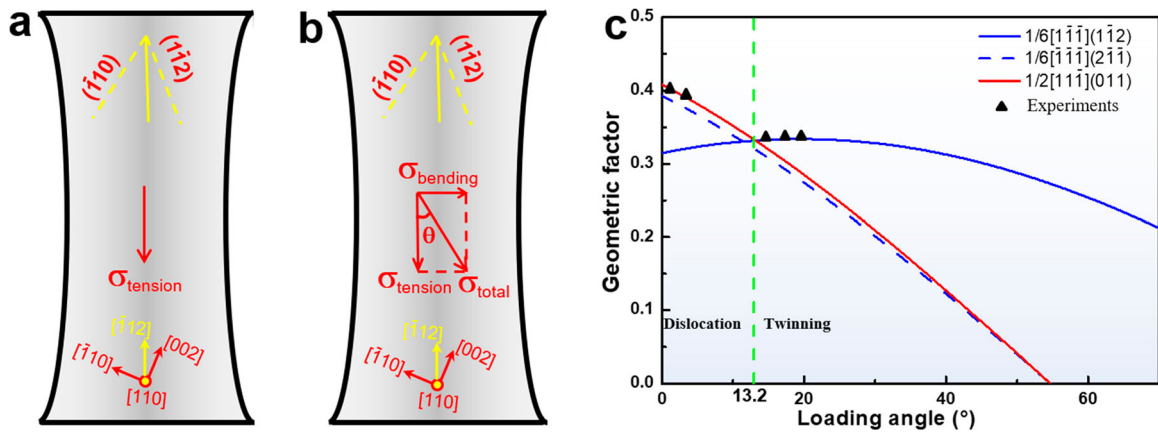


Figure 4. Schematic diagram of the stress status in $\langle 112 \rangle$ -oriented W nanowires under (a) uniaxial tensile loading and (b) the non-uniaxial loading of combined bending and tension. The yellow dashed lines represent the slip planes. (c) Largest geometric factors of twinning and dislocation slip as the function of the angle between the loading direction and the nanowire axis.

larger than that of dislocation slip, favoring the deformation twinning. In real experiments, we also deliberately conducted different tensile testing by controlling the angles between the loading direction and the nanowire axis to study the effect of loading angle on the deformation. Clearly, a transition from dislocation activity to deformation twinning did occur if the loading angle is higher than 13.2° (Figure 4(c), the black triangles represent samples tested with different loading angles, which are 2° , 4° , 14° , 17° and 19° , respectively). These observations are consistent with our analysis that the corresponding σ_{total} should be located within the twinning region under the non-uniaxial loading of combined bending and tension in Figures 2–3, favoring the deformation twinning.

It is also noticed that the morphology of deformation twinning formed under the uniaxial loading [12] and non-uniaxial loading [4,17] are different. Specifically, deformation twinning usually possesses relatively-flat twin boundaries under the uniaxial loading [10,12]; however, deformation twins formed under non-uniaxial loading typically show stepwise twin boundaries [17,25], which are composed of numerous $\{112\}$ atomic facets (Figure 3). The formation of such stepwise twin boundary with $\{112\}$ facets probably originated from the stress gradient caused by the loading geometry. Under uniaxial loading, the stress states in nanowire are uniform, making the energy barrier the dominating factor governing the deformation. However, the non-uniaxial loading (e.g. bending) can induce a significant stress gradient in the interior of nanowire, making the nanowire under non-uniform stress states [30]. This stress gradient causes a phenomenon that the resolved shear stresses on (112) twin planes (the driving force of twin nucleation and growth) is higher on one side of the nanowire than the stress on the other in the transverse direction [17]. Consequently, the formation of deformation twinning in $[112]$ -oriented W nanowires under non-uniaxial loading is mediated by the sliding of $1/6 \langle 111 \rangle$ twinning dislocation on $\{112\}$ planes, but the twinning width along the transverse direction of nanowire is different due to the existence of high stress gradient, resulting in a non-uniform twin thickness with stepwise twin boundaries composed of the $\{112\}$ atomic facets (see the zoomed-in image in Figure 3(d)). We notice that although the actual twin plane in BCC metals is $\{112\}$, the projection of stepwise twin boundaries with numerous $\{112\}$ atomic facets may show an illusion of overall $\{110\}$ interface when viewed along $[111]$ direction (Figure 2(b)). Similar twinning phenomenon was also observed in a recent molecular dynamics simulation study of bent $[100]$ α -Fe nanowires [17], which should be considered during the twin analysis in BCC metals. Our results present a direct

observation of such uncommon twinning behavior and twin boundary structure in the experiment, calling for an attention about the deformation twinning under complex stress state [15, 17]; however, further investigation about the magnitude of stress gradient needs to be conducted quantitatively.

In conclusion, the deformation of $\langle 112 \rangle$ -oriented W nanowires under the non-uniaxial loading is investigated using well-designed *in situ* TEM experiments. Dislocation plasticity dominates the deformation of $\langle 112 \rangle$ -oriented W nanowires under the uniaxial loading, while deformation twinning prevails in the nanowire under the non-uniaxial loading. This loading mode induced deformation transition is controlled by the critical resolved shear stress on the slip planes. Our experimental observations further reveal that the interfaces of bending-induced twinning are composed of numerous stepwise $\{112\}$ twin boundaries, the projection of which shows as an overall interface on $\{110\}$ when viewed in $\langle 111 \rangle$ zone axis. This uncommon behavior is attributed to the shear stress gradient induced by the non-uniaxial stress. This work reveals distinct deformation modes of $[112]$ -oriented W nanowires under different loading modes, shedding new light on the deformation mechanism of BCC nanocrystals under complex stress conditions.

Disclosure statement

No potential conflict of interest was reported by the authors.

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