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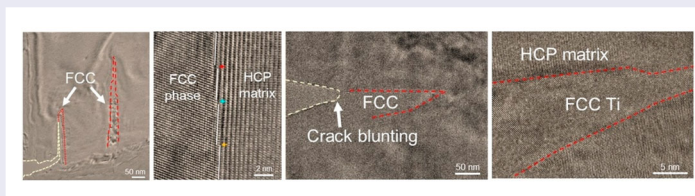
In situ TEM observation of HCP to FCC transitions in hexagonal close-packed titanium

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ABSTRACT

It remains controversial as to whether a face-centered cubic (FCC) phase exists in pure titanium (Ti) upon deformation, since the FCC structures in deformed Ti may well be TiH_x resulting from the sample preparation process. Here, by using in situ transmission electron microscopy (TEM), we uncover direct evidences on the nucleation and growth of FCC-Ti right in front of the crack tip in the α -Ti matrix. Atomic resolution images further reveal that the transformation can be mediated by either partial dislocations on basal planes or shear and atomic shuffle on the $\text{FCC } 1\ 1\ 0|\text{HCP } 1\ 0\ -1\ 0$ interfaces.



IMPACT STATEMENT

FCC-Ti's formation in pure α -Ti through deformation is controversial. In situ TEM observed FCC-Ti nucleation and growth in α -Ti matrix near the crack tip and revealed the mechanism.

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HCP-FCC transition;
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With excellent specific strength, titanium alloys are widely used in aerospace industries [1]. Phases of Ti alloys are critically associated with their mechanical performances [2–4]. Commercial pure Ti has a hexagonal close-packed (HCP) structure at room temperature commonly known as α -Ti. Upon heating and/or under pressure, titanium can transform into body-centered cubic, orthorhombic, trigonal, or hexagonal structures [5,6]. In certain cases, FCC-structured Ti has been observed in heat-treated [7,8] and deformed samples [9–14], Ti/Al and Ti/Ag multilayers [15–18], as well as in thin films of Ti on NaCl or Al substrate [19,20]. The formation of FCC-structured Ti is often attributed to deformation [9,21], alloying [22,23], and nonmetallic interstitial atoms [24,25]. Within these cases, two types of orientation relationships between the FCC and HCP-structured

Ti were reported: one is $\langle \bar{1}\ 2\ \bar{1}\ 0 \rangle_{\text{HCP}} || \langle 1\ \bar{1}\ 0 \rangle_{\text{FCC}}$ and $\{10\bar{1}0\}_{\text{HCP}} || \{110\}_{\text{FCC}}$ (so-called P-type); the other is $\langle \bar{1}\ 2\ \bar{1}\ 0 \rangle_{\text{HCP}} || \langle 1\ \bar{1}\ 0 \rangle_{\text{FCC}}$ and $\{0001\}_{\text{HCP}} || \{\bar{1}\bar{1}1\}_{\text{FCC}}$ (so-called B-type) [26–29].

However, the formation of titanium hydride (TiH_x) could also occur via hydrogen diffusion during mechanical grinding or TEM sample processing [30–32]; since TiH_x may also adopt an FCC structure that appears identical to the FCC-Ti in high-resolution TEM (HRTEM) images [33–35], there have been reports speculating that the FCC-Ti phases previously reported could potentially be titanium hydrides [6,30,36–39]. For instance, Chang *et al.* analysed the crystal structure and chemical composition of the FCC phase in electrochemically polished pure titanium and identified it as TiH_x [6]. Density functional calculations suggested that other nonmetallic interstitial

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atoms O, N, C, and B might also lead to the formation of FCC phase in Ti [24,25]; such effect of O has been well-demonstrated in experiments [36,39].

To explore the existence of FCC-structured Ti, in situ studies have been carried out trying to capture the HCP-to-FCC transition in Ti [40–43]. HCP-to-FCC transformations were captured in Ti thin films during in situ TEM heating at 600°C [40], and in nanosized Ti precipitates in a Nb-Ti-Si based alloy upon heating at 850°C [42,43]. Nonetheless, compelling evidence for the formation of FCC-Ti during deformation is still scarce.

Here, through in situ TEM tensile tests on pure Ti, we captured the nucleation and large-scale growth of FCC-Ti during deformation at room temperature, providing direct explicit evidences on the HCP-to-FCC transformation in Ti. Two interfacial processes of partial dislocation climbing and atomic shuffling associated with the B-type FCC and P-type FCC-Ti transformations were captured. Though both mechanisms contributed to the plastic deformation ahead of the crack tip, they interplayed with the crack propagation in different ways. Note that pre-existing FCC phase (likely TiH_x) was also captured which remained roughly the same in size when a crack approached and penetrated it.

Figure 1(a–e) and Supplementary Video 1 show a series of in situ TEM snapshots which demonstrate a nucleation and growth process of multiple FCC-Ti domains in front of a crack tip. The crack was experiencing a mode I loading along the $[1\ 0\ \bar{1}\ 0]$ direction of the HCP matrix. Due to the lack of deformation carriers, the straining in the vicinity was apparently mediated by the nucleation of a needle-shaped FCC phase (as indicated by the arrows in Figure 1(a–b)), which continuously extend along the $[1\ 0\ \bar{1}\ 0]$ direction with increasing loading. The orientation relation between the two phases was $\langle \bar{1}\ 2\ \bar{1}\ 0 \rangle_{\text{HCP}} \parallel \langle 1\ \bar{1}\ 0 \rangle_{\text{FCC}}$ and $\{0\ 0\ 0\ 1\}_{\text{HCP}} \parallel \{ \bar{1}\ \bar{1}\ 1 \}_{\text{FCC}}$, as shown in the HRTEM image of the FCC/HCP interface. Based on in situ observation (see Supplementary Video 2), the transformation was mediated by the partial dislocations on the interface, the gliding of which transformed the basal planes of the HCP matrix into the $\{1\ \bar{1}\ 1\}$ planes of the FCC phase in a layer-by-layer manner. Note that this mechanism was widely reported in HCP metals [26,40,41,43]. Continuous growth of the FCC phase in such a way effectively blunted and hence temporarily arrested the crack tip (Figure 1(b–d)). Meanwhile, it appeared that the FCC/HCP interface was sufficiently weak that it was teared apart by the normal stress on the interface; the attendant crack path was diverted (Figure 1(d–e)).

Figure 2(a) shows a propagation process of another crack that is experiencing stress loaded along the $[50\bar{1}1]$ direction of the HCP matrix. The FCC-Ti nucleated with the crack propagation and grew approximately

parallel to the initial direction of crack extension (Figure 2(b–e)). Based on the HRTEM image in Figure 2(f), the longitudinal boundaries between the FCC and HCP phases were parallel to the $\{1\ 0\ \bar{1}\ 0\}$ plane, the orientation relation between the two phases in this case was $\langle \bar{1}\ 2\ \bar{1}\ 0 \rangle_{\text{HCP}} \parallel \langle 1\ \bar{1}\ 0 \rangle_{\text{FCC}}$ and $\{10\bar{1}0\}_{\text{HCP}} \parallel \{1\bar{1}0\}_{\text{FCC}}$. Furthermore, a series of enlarged HRTEM snapshots revealed that the growth of the FCC phase was actually carried by layer-by-layer transformation of the prismatic planes in the HCP matrix into the $\{1\bar{1}0\}$ planes in the FCC-Ti (see Figure 3). The in situ HRTEM observations provide direct evidence for the HCP-to-FCC transformation mechanism associated with the P-type FCC-Ti [27,44–46]. Note that, similar to the case in Figure 1, the crack tip also blunted as the FCC-Ti grew and diverted its path in subsequent loading (Supplementary Video 3).

To exclude the possibility of TiH_x , we conducted electron energy loss spectroscopy (EELS) analysis on the FCC phase observed during the in situ experiments, as illustrated in the Figure 4. By comparing the EELS spectrums of the HCP matrix and the as-formed FCC phase, no discernible peak at 13 eV for hydrogen (H) was observed, evidencing no substantial presence of H in the FCC phase. This key finding further confirms that the FCC phase observed at the crack tips is indeed a deform-induced FCC-Ti phase. Moreover, to eliminate the potential influence of H on the formation of FCC-Ti phase, we repeated the in situ tensile experiment by using ion-milled Ti samples (see appending Methods for details), avoiding the introduction of H during the sample preparation. Consistent with our previous observations, the FCC-Ti phases were again observed near the cracks, as shown in Figure 4(c–d). Notably, the absence of peak for H (at 13 eV) in the EELS spectra of FCC-Ti or matrix. These results further confirmed that the deform-induced FCC-HCP transformation mechanism in Ti.

Note that pre-existing FCC phases which was likely TiH_x was also spotted. This is reasonable since the TEM sample was made by conventional twin-jet electrochemical polishing process which was known to incur the TiH_x . It has been challenging to prevent the occurrence of hydrogen and hydrides during sample processing and observation, as reported previously [6]. Figure 5(a–d) unveils its response upon straining and interplay with the crack propagation. A needle-shaped FCC phase was present at the beginning and remained almost unchanged during the entire crack extension process. The crack extended through the FCC phase and into the HCP matrix, while maintaining its direction. EELS analysis also clarified the presence of TiH_x , as shown in Figure 5(e–g).

This observation is reasonable since the growth of TiH_x in principle requires a continuous feeds of

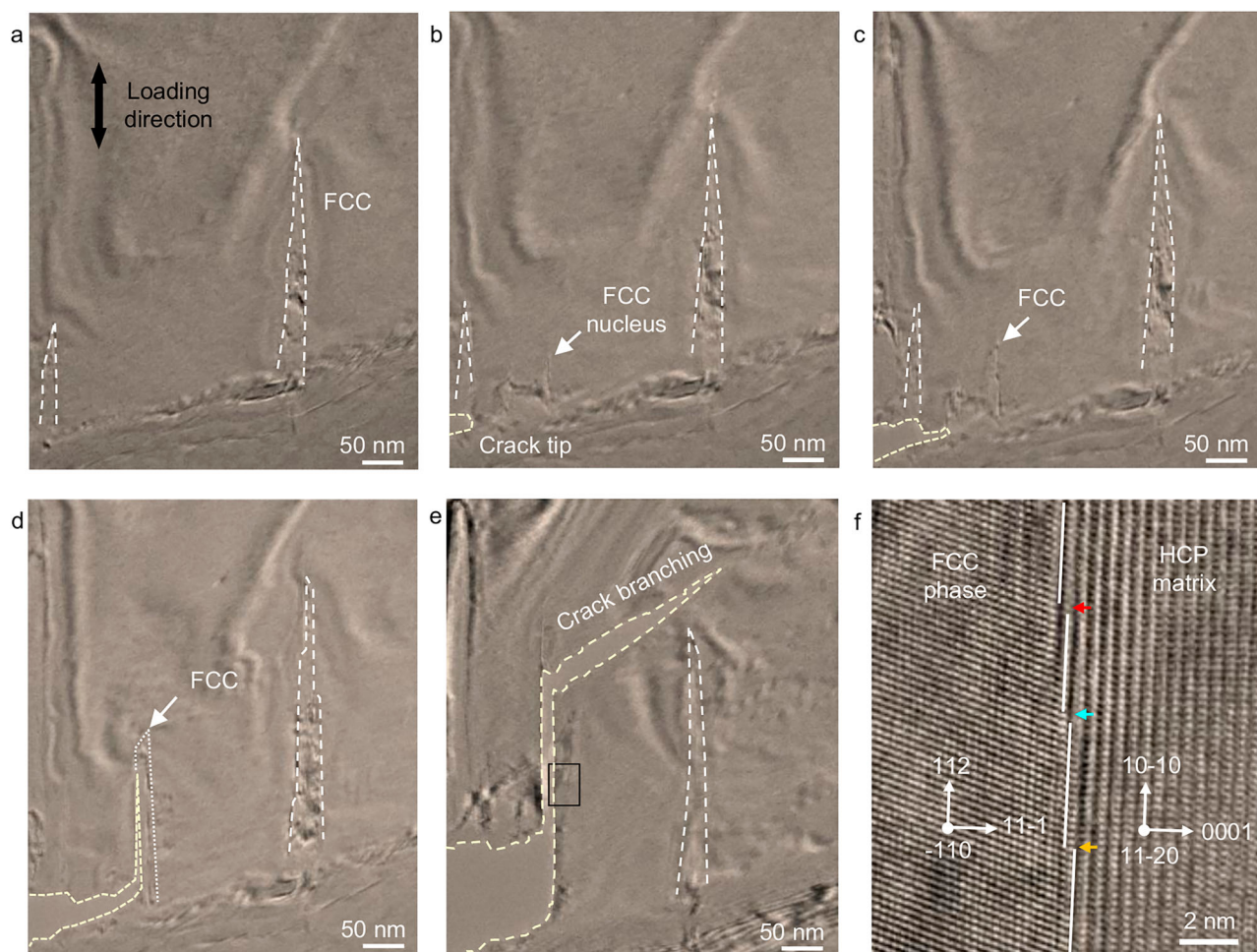


Figure 1. Sequential in situ TEM snapshots showing the nucleation and growth of FCC Ti phase in front of a crack tip (a–e). (f) HRTEM snapshot of the interface between the B-type FCC-Ti and the HCP matrix.

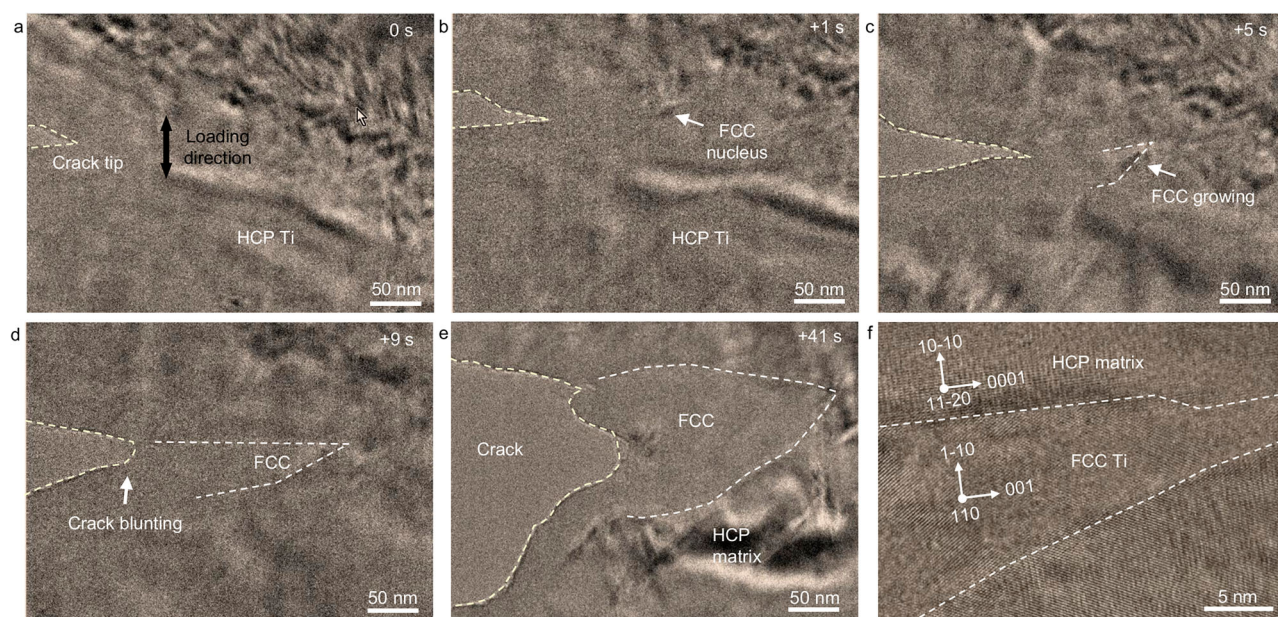


Figure 2. Sequential in situ TEM snapshots on the nucleation and growth of P-type FCC-Ti ahead of a crack tip (a–e). (f) HRTEM snapshot of the interface between the P-type FCC-Ti and the HCP matrix.

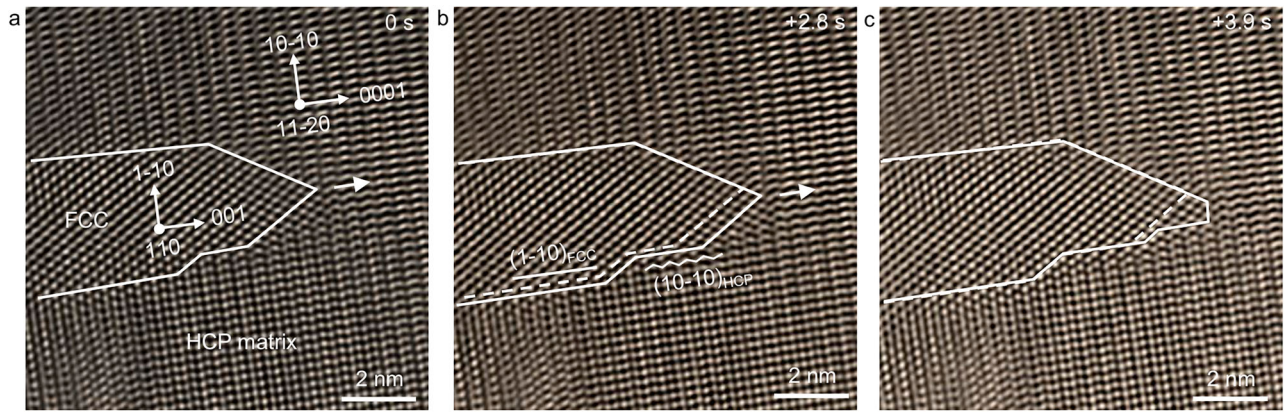


Figure 3. Sequential HRTEM snapshots of the atomic shuffling process that mediated the growth of the P-type FCC-Ti in the HCP matrix. The solid lines represent the interfaces, while the dash lines indicate the interface position in the prior snapshot.

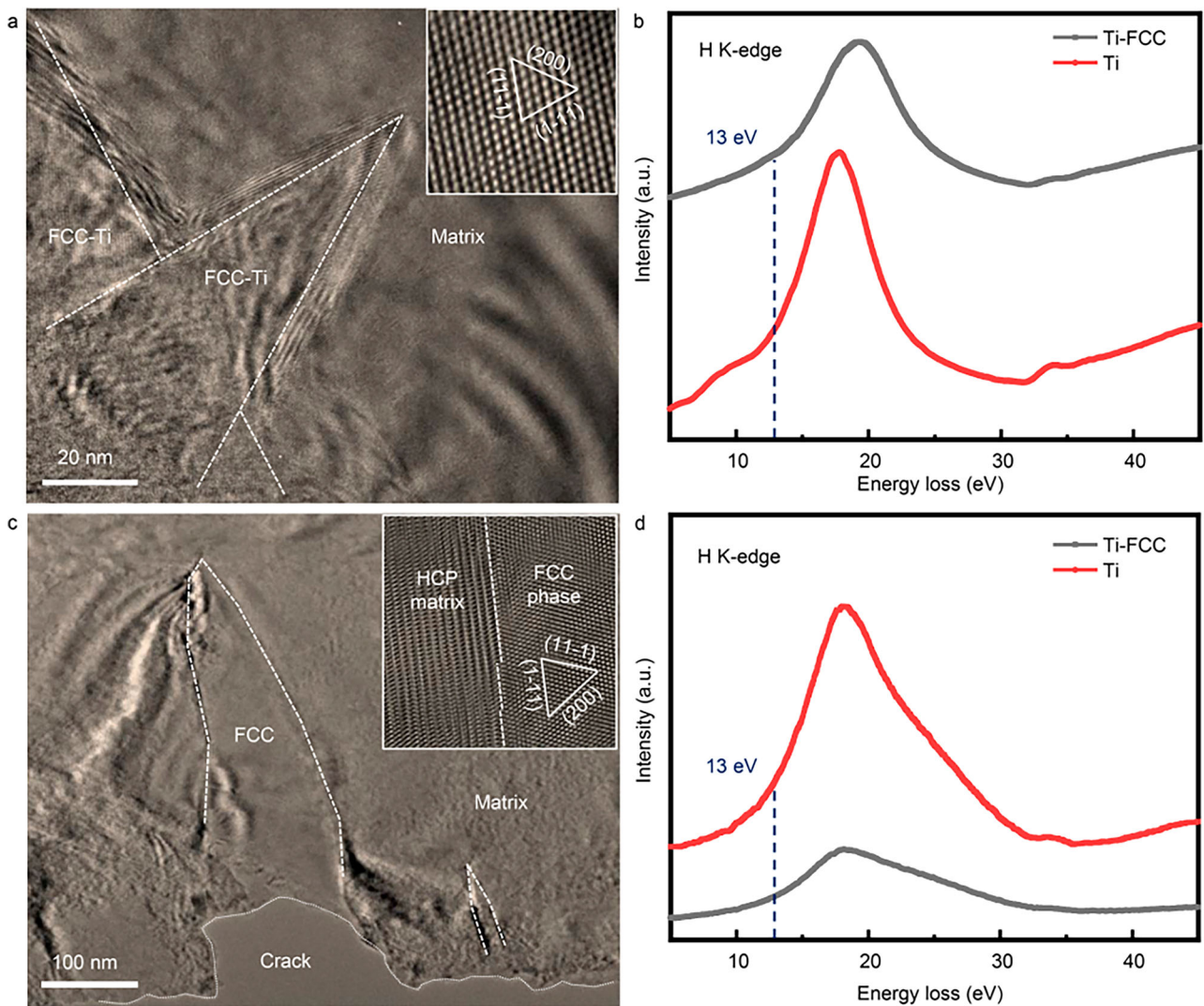


Figure 4. HRTEM images and electron energy loss spectroscopy (EELS) analysis of the deform-induced FCC-Ti. (a) TEM image of the FCC-Ti, and inset is an HRTEM image of FCC-Ti. (b) EELS spectrums obtained from the FCC-Ti phase (black line) and the matrix Ti (red line). The sample was prepared by twin-jet electropolishing. (c) TEM image of the FCC-Ti, and inset is an HRTEM image of FCC-HCP interface. (d) EELS spectrums obtained from the FCC-Ti phase (black line) and the matrix Ti (red line). The sample was prepared by dry-polishing and ion-milling.

hydrogen atoms. Although the relatively high tensile strain can prompt hydrogen aggregation in the vicinity of the crack tip, the high energy barrier for hydrogen atom diffusion in the HCP-structured Ti matrix makes hydrogen diffusion difficult. Referring to first-principles

calculations, the energy barrier of hydrogen diffusion in α -Ti and TiH_x is more than 0.5 eV (even 0.94 eV of TiH_2) which is far beyond the thermal activation at room temperature [47,48]. This, in turn, prevents the rapid growth of titanium hydrides in response to tensile strains

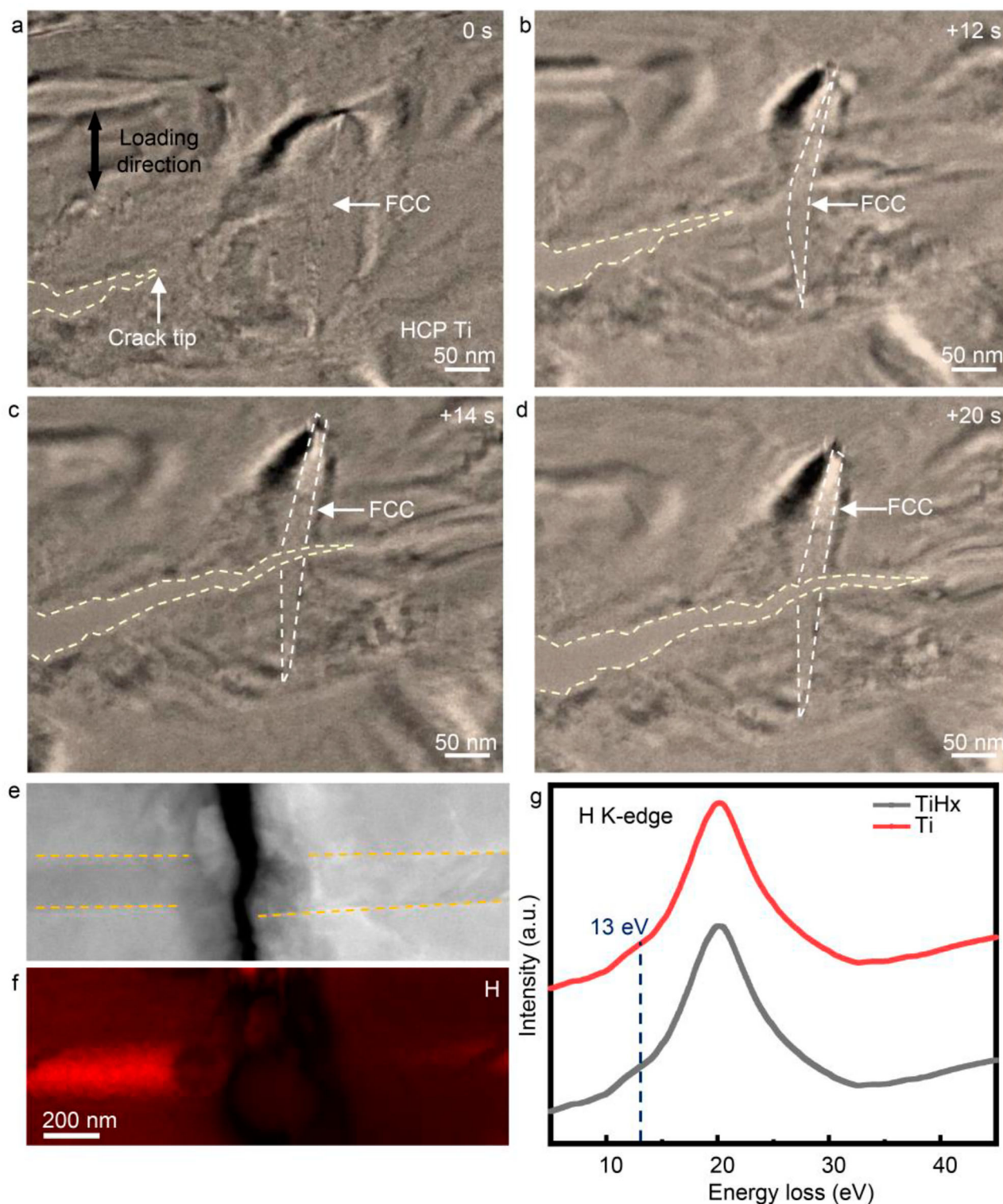


Figure 5. TEM and EELS analysis on the titanium hydride domains. (a–d) Sequential TEM snapshots on a crack propagation process through a titanium hydride domain (outlined by the white dash lines). (e–f) STEM image and EELS mapping of H of the TiH_x lamella, featuring with an enrichment of H. (g) EELS spectra obtained from the FCC-structured TiH_x (black line) and the matrix Ti (red line).

and hence explains the trivial growth of the FCC phase in Figure 5.

To recap, the above in situ findings demonstrate that deform-induced HCP-to-FCC phase transition does exist in pure Ti. The nucleation and growth of B-type and P-type FCC-Ti were captured in front of the propagating crack tip in pure α -Ti at room temperature. The study further reveals the roles of the FCC phase in cracking; the HCP-to-FCC transition could blunt the crack tip and hence release the stress concentration in the region. Such a transformation may also contribute to the deformation at the crack tip especially when facile deformation modes are scarce. The weak interface between the B-type FCC phases and HCP matrix could induce cracking along the FCC/HCP interface and hence alter the crack propagation direction.

Methods

Commercial pure titanium (99.9% purity) was used for the in situ TEM tensile tests. Some TEM samples were prepared by mechanical polishing to a thickness of 80 μm and then twin-jet electropolishing in an etching solution of 6% perchloric acid and 94% methanol at -35°C . Additionally, to avoid hydrogen during the sample preparation process, some TEM samples were also prepared by mechanical grinding without water or alcohol to 50 μm and then Ar-milling in a Fischione Model 1051 system. The in situ TEM tensile tests were conducted on an aberration-corrected TEM (Spectra 300, Thermo Fisher Scientific) using a Gatan Model 654 single-tilt straining holder. The images were recorded using a charge-coupled device. EELS was acquired with a Gatan GIF Continuum 1065 instrument.

Disclosure statement

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

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