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Mechanisms for deformation induced hexagonal close-packed structure to face-centered cubic structure transformation in zirconium

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ABSTRACT

Two distinctive orientation relations between hexagonal close-packed (HCP) phase and face-centered cubic (FCC) phase were observed simultaneously in cold-rolled pure Zr, which were denoted as B-type and P-type orientation relations according to whether the phase interface is parallel to the basal plane or prism plane of the HCP matrix. The mechanisms for the phase transformation generating the two different HCP-FCC orientation relations were thoroughly analyzed. B-type orientation relation was achieved when HCP to FCC phase transformation occurred via collective gliding of Shockley partial dislocations on basal planes, while P-type orientation relation was attained through pure-shuffle and shear-shuffle mechanisms.

The transformation from a hexagonal close-packed (HCP) structure to a face-centered cubic (FCC) structure has been widely observed in metals and alloys [1–12]. The HCP to FCC phase transformation typically produces two different orientation relations between the two phases: (1) $\langle 1\bar{2}10\rangle_{HCP}//\langle\bar{1}10\rangle_{FCC}$ and $\{0001\}_{HCP}//\{\bar{1}11\}_{FCC}$, (2) $\langle 0001\rangle_{HCP}//\langle 001\rangle_{FCC}$ and $\{10\bar{1}0\}_{HCP}//\{220\}_{FCC}$. In the former one, the longitudinal boundary between two phases is parallel to the {0001} plane, basal plane of the HCP matrix. Therefore, this phase transformation and the resultant orientation relation can be denoted as B-type phase transformation and B-type orientation relation, which has been observed in Ti-based alloys [1–3], Hf [4], Co [5,6], InAs nanowires [7] and stainless steel [8,9]. In the latter one, the longitudinal boundary between the two phases is parallel to the $\{10\bar{1}0\}$ plane, which is the prism plane of the HCP matrix. Thus, this phase transformation and the resultant orientation relation can be denoted as P-type phase transformation and P-type orientation relation, which has been observed recently in pure Ti after plastic deformation [10–12].

For B-type transformation, it is reported that the gliding of Shockley partials on every other {0001} basal planes in HCP matrix can result in the HCP stacking sequence…ABAB…transforming to the FCC sequence…ABCABC… [4,7–9]. For P-type transformation, Hong et al. [10] and Ren et al. [12] proposed that Shockley partials gliding on every other $\{10\bar{1}0\}$ prism planes in HCP matrix can trigger the P-type phase transformation. However, Wu et al. [11] proposed a different mechanism that the P-type transformation is accomplished by pure-shuffle and shear-shuffle mechanisms, instead of partial dislocation gliding. It can be seen from literatures that, the B-type phase transformation was commonly seen in various materials and partial dislocation gliding was widely accepted as the transformation mechanism, while the P-type phase transformation was only reported in pure Ti till recently and discrepancy still exists as to the transformation mechanism. In the present study, we report the observation of both B-type and P-type HCP-FCC transformations in bulk cold rolled Zr for the first time. Through detailed high-resolution TEM (HRTEM) analysis, we elucidated the mechanisms for both B-type and P-type transformations at atomic scale.

The materials used in this study are commercially pure Zr (99.99 at.%). The as-received materials show an equiaxed grain structure with the grain size ranging from 20 μm to 30 μm. Small bars with a dimension of 30 mm × 10 mm × 3 mm were cut from the as-received plates. These small bars were sealed in high vacuum tubes and annealed for 1 h to eliminate deformation history, and then were cold-rolled at room temperature multiple times with a thickness reduction of 0.3 mm per pass to eventually reach a total thickness reduction of 60%.

The TEM specimens cut from normal plane were first ground into 80 μm and then punched into discs with a diameter of 3 mm. These discs were further thinned using a double-jet electrolytic polisher (Struers TenuPol-5) and a solution of 10% perchloric acid + 90% methanol at −34 °C with an applied voltage of 10.5 V. The TEM specimens cut from the transverse plane were ground into 50 μm, dimpled and then Ar^{+} ion-milled using a Gatan 691 PIPS system with a voltage of 3 kV. TEM observations were performed using a FEI Titan G2 60-300 Cs-corrected microscope operated at 300 kV.

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Fig. 1 shows the typical TEM images and the corresponding selected area electron diffraction (SAED) patterns of the cold-rolled Zr with a thickness reduction of 60%. After rolling deformation, small lamellas were observed within the HCP matrix, as shown in Fig. 1a and c. Fig. 1b and d show HRTEM images of the rectangular areas as marked in Fig. 1a and c, respectively. Both SAED patterns and HRTEM images present the orientation relations between the lamella and the matrix. From Fig. 1b, the lamella is an FCC phase viewed from $\langle\bar{1}10\rangle$ axis and the orientation relation between the HCP matrix and FCC lamella is $\langle 1\bar{2}10\rangle_{HCP}//\langle\bar{1}10\rangle_{FCC}$ and $\{0001\}_{HCP}//\{\bar{1}11\}_{FCC}$. The longitudinal boundary between the two phases is parallel to the {0001} plane, the basal plane of the HCP matrix. Therefore this is the B-type phase transformation induced orientation relation. From Fig. 1d, the lamella also has an FCC structure, but the orientation relation between the HCP matrix and the FCC phase is $\langle 0001\rangle_{HCP}//\langle 001\rangle_{FCC}$ and $\{10\bar{1}0\}_{HCP}//\{220\}_{FCC}$. The longitudinal boundary between two phases is parallel to the $\{10\bar{1}0\}$ plane, the prism plane of the HCP matrix, so it is the P-type orientation relation.

Detailed HRTEM investigations were carried out to understand the phase transformation mechanisms. Fig. 2a shows an HRTEM image containing an FCC lamella with B-type orientation relation. Fig. 2b and c as inserted in Fig. 2a are the enlarged Fourier-filtered TEM images of the interfaces at two sides of the lamella on the same atomic planes. The atomic stacking sequences in the left and right regions in Fig. 2b are …ABAB… (HCP structure) and …ABCABC… (FCC structure), respectively. Three Burgers circuits based on the HCP lattice were drawn in the interface between the HCP and the FCC structures, showing three 30° Shockley partial dislocations on three (0001) planes (detailed explanations on how to identify the type of partial dislocations are provided in the literature [4]). In Fig. 2c, three Burgers circuits based on the HCP lattice were drawn, indicating two 30° and one 90° Shockley partials. Theoretically, Shockley partial dislocations typically stem from two possible sources: dissociations of ⟨a⟩ -type dislocations or dissociations of ⟨a + c⟩ -type dislocations. In the former case, both ends of the FCC lamella contain Shockley partials. In the latter case, at one end of the FCC band there must be many sessile dislocations [4]. In Fig. 2, there is no sessile dislocation locating at any side of the lamella, indicating that these phase transformation-related partials stemmed from the dissociation of ⟨a⟩ -type dislocations. A 60° mixed-type ⟨a⟩ dislocation can dissociate into a 30° mixed-type partial and a 90° pure edge partial, while a screw ⟨a⟩ dislocation can dissociate into two 30° mixed-type partials [13,14]. Need to mention that, the red line in Fig. 2 indicates the same atomic layer of the FCC lamella. Thus those Shockley partials, locating in the phase interface regions in Fig. 2b and c as indicated, derived from the dissociations of two screw ⟨a⟩ dislocations and one 60° mixed-type ⟨a⟩ dislocation. From the analysis mentioned above, the B-type HCP to FCC phase transformation can be realized by follows: Shockley partials with Burgers vectors of the $a/3\langle 10\bar{1}0\rangle$ type were generated and glided on (0001) plane during rolling deformation. Coordinated activation of these partials gliding on every other (0001) plane gradually converted the HCP structure to the FCC structure.

The P-type HCP to FCC phase transformation and the resultant orientation relation between the two phases were rarely observed in

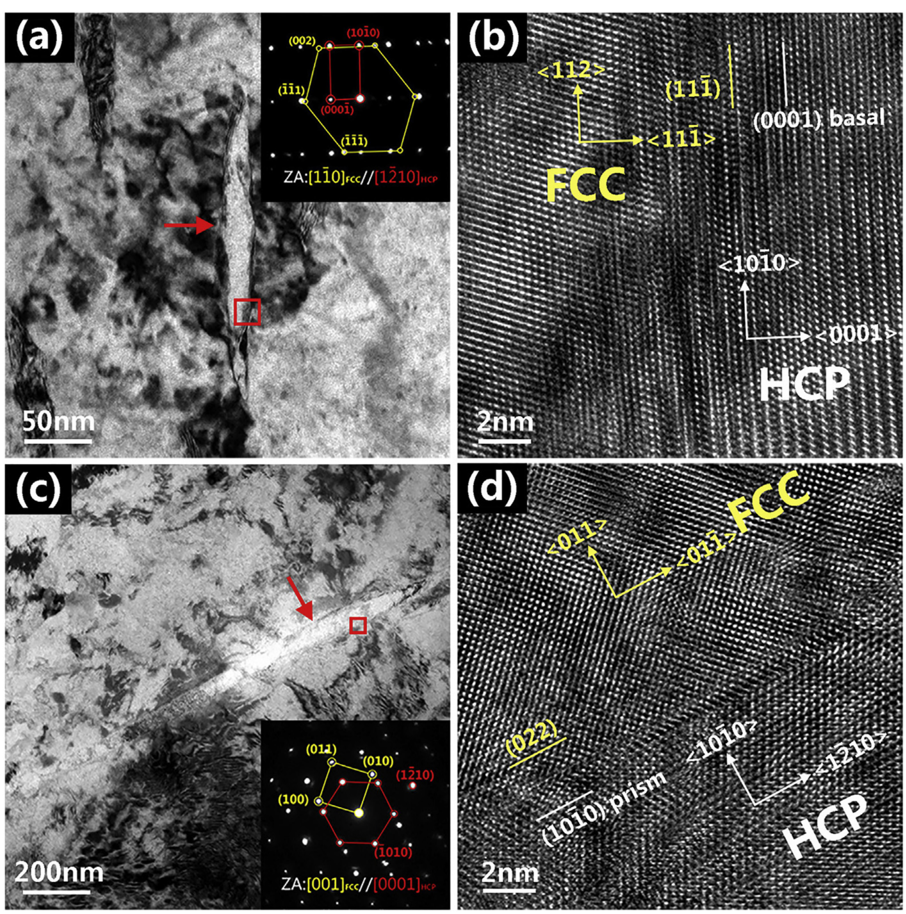

Fig. 1. (a) A TEM image and the corresponding SAED pattern of the cold-rolled Zr with a thickness reduction of 60%. (b) An HRTEM image of the red rectangular area in (a), showing the longitudinal HCP-FCC phase interface is parallel to the {0001} basal plane. (c) Another TEM image and the corresponding SAED pattern of the cold-rolled Zr. (d) An HRTEM image of the red rectangular area in (c), showing the longitudinal HCP-FCC phase interface is parallel to the $\{10\bar{1}0\}$ prism plane. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)