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Formation and Characterization of CuPt-A type Ordered Structure in Cadmium Zinc Telluride Single Crystals

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Supporting Information

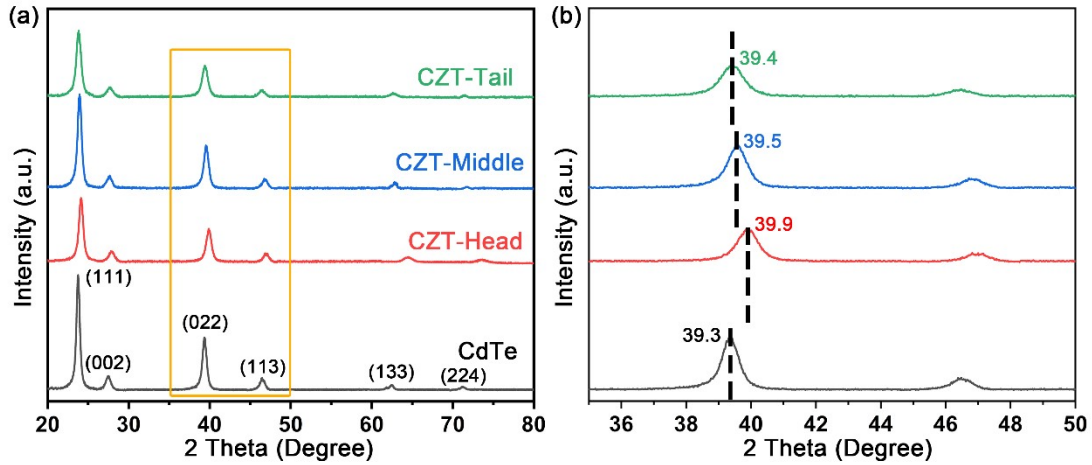

Figure S1 The powder XRD spectra (a) and partial enlarged position of CdTe and CZT single crystals taken from different parts suggest the different lattice parameters.

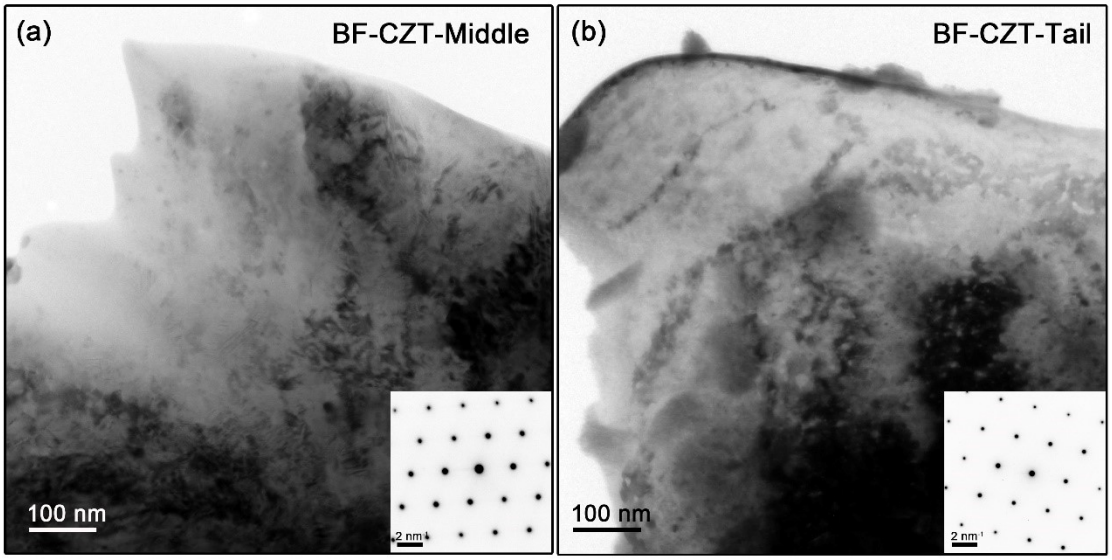

Figure S2 TEM BF image and corresponding SAED patterns of the CZT sample taken from middle (a) and tail part (b) of the ingot illustrates the excellent crystallinity and single disordered phase nature.

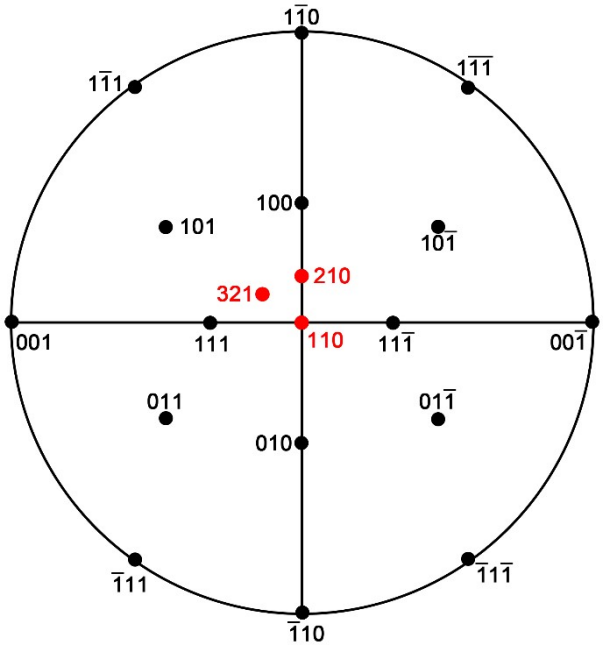

Figure S3 The stereographic projection of vectors illustrates the 3 different viewing directions (marked with red color) achieved through TEM series tilting experiment.

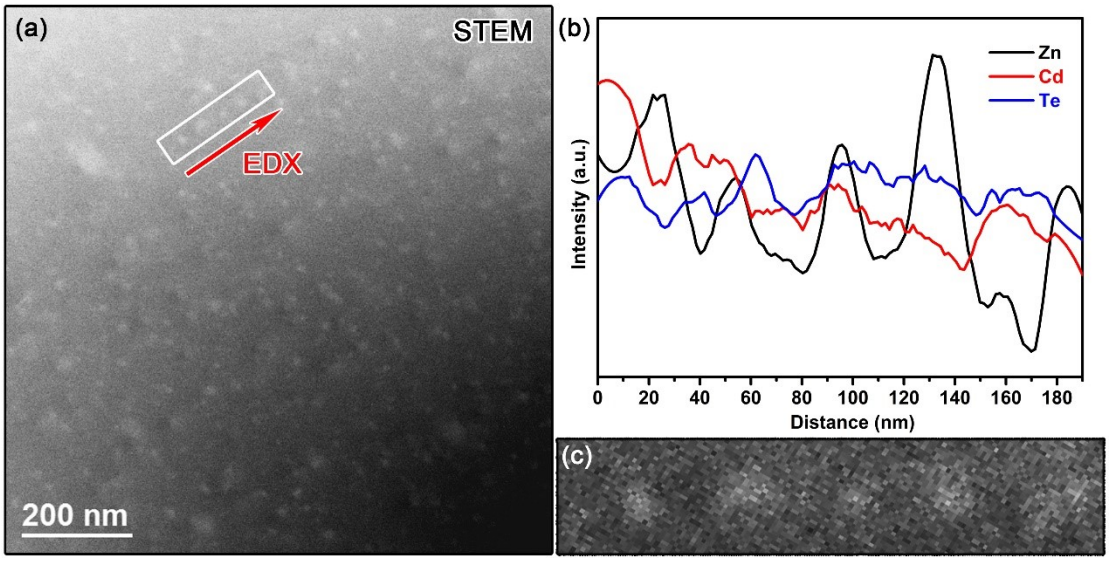

Figure S4 STEM BF image (a) and corresponding EDX line scan results (b, c) suggest the local enrichment of Zn element at the position of the ordered phase particles.

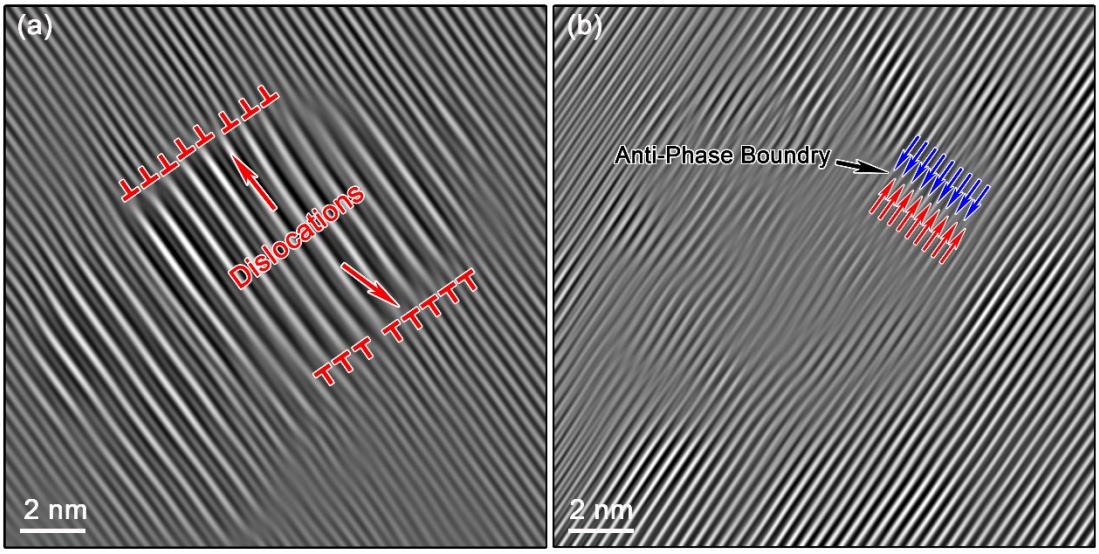

Figure S5 The IFFT images taken from the area enclosed by the red dashed line in Figure 3 (a) by using $(h\bar{h}h)$ and $(\bar{h}hh)$ series of spots clearly illustrate the existence of regularly arranged dislocations and anti-phase boundaries at the interface between ordered and disordered phases.

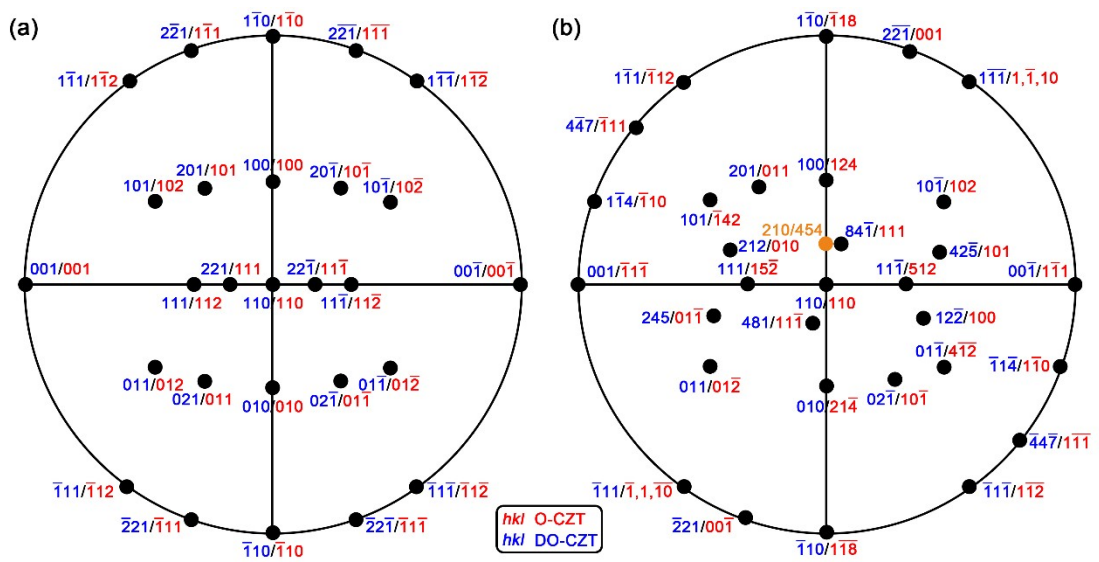

Figure S6 The stereographic projection diagrams of planes for variant 1 (a) and variant 2 (b) illustrate the totally different orientation relationships (ORs). Rotating the projection diagram of the OR between the variant 1 and the substrate clockwise by 109.5° along the direction of the projection center can achieve projection diagram of OR between the variant 2 and the substrate.

Table S1 The angle data recorede from the goniometer system of TEM

Viewing Direction	TX	TY	Tilting Angle from OR-I (θ)	Orientation Difference with [110]
VD-I-[110]	4.6	-0.6	0°	NA
VD-II-[210]	17.3	13.5	18.9°	18.4°
VD-III-[321]	-14.7	-2.5	19.4°	19.1°