Compared to α-Titanium alloys (Hexagonal), β-Titanium alloys (BCC) are inherently ductile and have promising potentials to substitute new technology materials in daily life. Mo is commercially added as β-Ti stabilizer to precipitate finely dispersed round shaped α-Ti phase in the β-Ti matrix to enhance the hardness of the Titanium. Interestingly, this α-Ti precipitate is not nucleated directly from the β-Ti phase but from the nucleation sites provided by ω precipitates. Though there have been intensive studies on the phase transformation of β → α, detailed atomistic dynamics, including the ω phase, have rarely been investigated. We study Ti-Mo(15 wt%) alloy for the phenomena of α-Ti phase formation from the ω precipitate using aberration corrected high annular angle dark field scanning electron transmission microscopy (HAADF-STEM) and electron energy loss spectroscopy for chemical information as well as atomic structural information. We present direct images of the early stage in ω → α transition state exhibiting a metastable state. In bright and dark Z-contrast regions of ω precipitates, the atomic arrangement as well as Z-contrast seems very different from each other. Bright Z-contrast regions show an atomically resolved projected image of ω precipitate crystal structure in the [112̅0] zone axis (Fig. 1B), while dark Z-contrast regions show a burry image which is not easy to be interpreted. The image of dark Z-contrast region has a layered periodic pattern and the atoms on each layer are not well resolved as presented in Fig. 1A. The Ti atomic layers could be considered as a metastable phase which will finally develop to a part of α precipitate. We speculate that the metastable structure is formed by distortions caused by local defects of the ω phase. Substantial amount of stacking faults and dislocations in an extremely early stage of ω → α phase transition supports this hypothesis. Using systematic ab-initio calculations, we found that there is a reasonably stable defective ω-Ti structure which is relaxed to the structure similar to the Z-contrast in HAADF-STEM images (Fig. 2). It is also confirmed that the defective Ti structure is relaxed to the stable hexagonal α-Ti structure with additional Ti atoms on the Ti deficient sites, converting the [112̅0]ω phase orientation to [0001]α directly. This study demonstrates that ω → α transition in Ti-Mo alloy system is governed by defect mediated phase transformation.

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Fig. 1: Enlarged HAADF-STEM image of [11-20]ω//[110]β orientation in rapidly cooled Ti-15wt% Mo sample after aging at 400°C. The Z-contrast of region A is apparently different from the atomic array of ω phase in region B.

Fig. 2: Position of considered layered defects (left) and the Ab-initio calculation result of fully relaxed structure with defects (right).