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Ti $\alpha-\omega$ phase transformation and metastable structure, revealed by the solid-state nudged elastic band method[1] NIKOLAI ZARKEVICH[2], DUANE D. JOHNSON[2,], Ames Laboratory — Titanium is on of the four most utilized structural metals, and, hence, its structural changes and potential metastable phases under stress are of considerable importance. Using DFT+U combined with the generalized solid-state nudged elastic band (SS-NEB) method, we consider the pressure-driven transformation between Ti α and ω phases, and find an intermediate metastable body-centered orthorhombic (bco) structure of lower density. We verify its stability, assess the phonons and electronic structure, and compare computational results to experiment. Interestingly, standard density functional theory (DFT) yields the ω phase as the Ti ground state, in contradiction to the observed α phase at low pressure and temperature. We correct this by proper consideration of the strongly correlated d-electrons, and utilize DFT+U method in the SS-NEB to obtain the relevant transformation pathway and structures.

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[2]Ames Laboratory, U.S. Department of Energy at Iowa State University, Ames, Iowa 50011-3020

Nikolai A. Zarkevich
Ames Laboratory

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